

(FILE 'HOME' ENTERED AT 10:58:37 ON 24 SEP 2008)

FILE 'REGISTRY' ENTERED AT 10:58:48 ON 24 SEP 2008

L1 STRUCTURE UPLOADED  
L2 68 S SSS L1 FULL

FILE 'CAPLUS' ENTERED AT 10:59:12 ON 24 SEP 2008

L3 117 S L2  
E KIDNEY+ALL/CT  
E NEPHRITIS+ALL/CT  
E GLOMERULONEPHRITIS+ALL/CT  
L4 4 S L3 AND (KIDNEY OR RENAL OR NEPHRO? OR NEPHRITIS OR GLOMERULON  
L5 100 S L3 AND PD <=2003  
L6 100 FOCUS L5 1-  
L7 0 S IBIB ABS HITSTR 1-100

=> d ibib abs hitstr 1-100 l6

L6 ANSWER 1 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:17915 CAPLUS  
DOCUMENT NUMBER: 106:17915  
ORIGINAL REFERENCE NO.: 106:3065a,3068a  
TITLE: Oxaluric acid derivatives and pharmaceutical compositions containing them  
INVENTOR(S): Ienaga, Kazuharu; Nakamura, Ko; Ishii, Akira  
PATENT ASSIGNEE(S): Nippon Zoki Pharmaceutical Co., Ltd., Japan  
SOURCE: Eur. Pat. Appl., 32 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 191735	A2	19860820	EP 1986-810068	19860210 <--
EP 191735	A3	19870204		
EP 191735	B1	19900912		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 61183259	A	19860815	JP 1985-24010	19850209 <--
JP 06060152	B	19940810		
US 4708954	A	19871124	US 1986-826997	19860207 <--
PRIORITY APPLN. INFO.:			JP 1985-24010	A 19850209

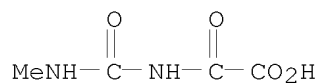
OTHER SOURCE(S): MARPAT 106:17915

AB The title compds. R1R2NCONHCOCO2R3 (I; R1, R2 = H, alkyl, cycloalkyl; R1R2N = heterocyclyl; R3 = H, alkyl) and their salts and metal complexes, useful in treatment of diabetes, were prepared. Thus, MeNHCONH2 in THF was reacted with (ClCO)2 to give 1-methylimidazolidinetrione which was stirred in N NH3 at room temperature to give I (R1 = Me, R2 = H, R3 = NH4) (II). In hyperglycemic rats II at 100 mg/kg, orally, reduced blood glucose levels by 25.2%. Pharmaceutical formulations containing I are presented.

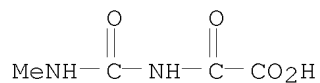
IT 89281-42-5P 105918-80-7P 105918-81-8P  
105918-82-9P, 5-Butyloxaluric acid 105918-83-0P  
105918-84-1P 105918-85-2P 105918-86-3P  
105918-87-4P 105918-88-5P 105918-89-6P  
105918-90-9P 105918-91-0P 105918-92-1P  
105918-93-2P 105918-94-3P 105918-97-6P  
105919-00-4P 105934-76-7P 105934-77-8P  
105934-78-9P 105934-79-0P 105934-80-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as antidiabetic)

RN 89281-42-5 CAPLUS

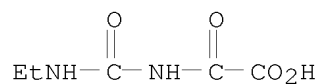
CN Acetic acid, 2-[[ (methylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



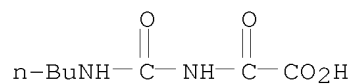
RN 105918-80-7 CAPLUS  
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 (CA INDEX NAME)



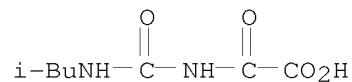
RN 105918-81-8 CAPLUS  
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 (CA INDEX NAME)



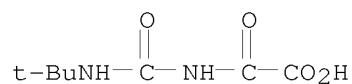
RN 105918-82-9 CAPLUS  
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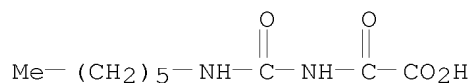
RN 105918-83-0 CAPLUS  
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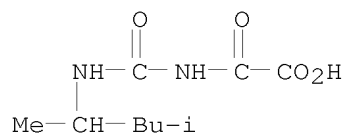
RN 105918-84-1 CAPLUS  
 CN Acetic acid, 2-[[ [(1,1-dimethylethyl)amino]carbonyl]amino]-2-oxo- (CA INDEX NAME)



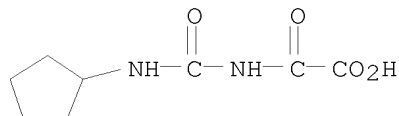
RN 105918-85-2 CAPLUS  
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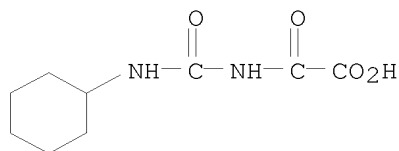
RN 105918-86-3 CAPLUS  
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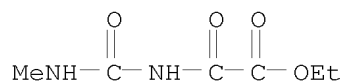
RN 105918-87-4 CAPLUS  
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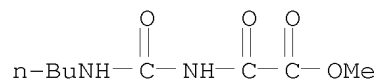
RN 105918-88-5 CAPLUS  
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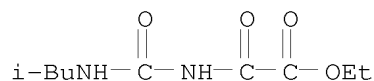
RN 105918-89-6 CAPLUS  
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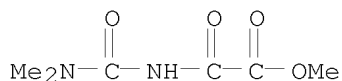
RN 105918-90-9 CAPLUS  
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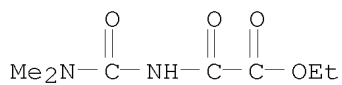
RN 105918-91-0 CAPLUS  
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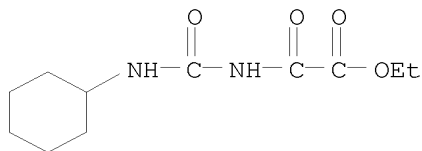
RN 105918-92-1 CAPLUS  
 CN Acetic acid, 2-[[ (dimethylamino)carbonyl]amino]-2-oxo-, methyl ester (CA INDEX NAME)



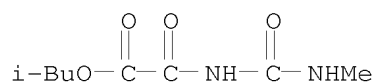
RN 105918-93-2 CAPLUS  
 CN Acetic acid, 2-[[ (dimethylamino)carbonyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)



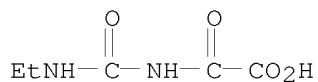
RN 105918-94-3 CAPLUS  
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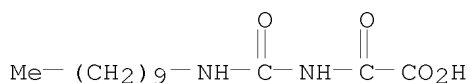
RN 105918-97-6 CAPLUS  
 CN Acetic acid, 2-[[ (methylamino)carbonyl]amino]-2-oxo-, 2-methylpropyl ester (CA INDEX NAME)



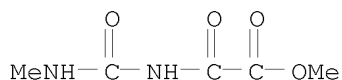
RN 105919-00-4 CAPLUS  
 CN Acetic acid, 2-[[ (ethylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



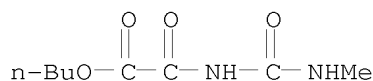
RN 105934-76-7 CAPLUS  
 CN Acetic acid, 2-[[ (decylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



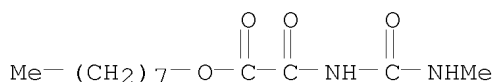
RN 105934-77-8 CAPLUS  
 CN Acetic acid, 2-[[ (methylamino)carbonyl]amino]-2-oxo-, methyl ester (CA INDEX NAME)



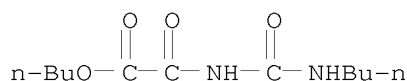
RN 105934-78-9 CAPLUS  
 CN Acetic acid, 2-[[ (methylamino)carbonyl]amino]-2-oxo-, butyl ester (CA INDEX NAME)



RN 105934-79-0 CAPLUS  
 CN Acetic acid, 2-[[ (methylamino)carbonyl]amino]-2-oxo-, octyl ester (CA INDEX NAME)



RN 105934-80-3 CAPLUS  
 CN Acetic acid, 2-[[ (butylamino)carbonyl]amino]-2-oxo-, butyl ester (CA INDEX NAME)



L6 ANSWER 2 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:100431 CAPLUS

DOCUMENT NUMBER: 130:237830

TITLE: Synthesis and biological activity of aryloxaluric acid derivatives

AUTHOR(S): Petyunin, G. P.; Chubenko, O. V.; Abdulatif, Alsouri

CORPORATE SOURCE: Khark. Inst. Udoskonalennya Likariv, Kharkov, Ukraine

SOURCE: Farmatsevtichnii Zhurnal (Kiev) (1997), (5), 42-45

CODEN: FRZKAP; ISSN: 0367-3057

PUBLISHER: Zdorov'ya

DOCUMENT TYPE: Journal

LANGUAGE: Ukrainian

OTHER SOURCE(S): CASREACT 130:237830

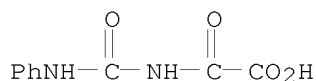
AB Aryloxaluric acid salts and amides with amino acids or glucosamine were prepared and shown to have antimicrobial and local anesthetic activities.

IT 221391-56-6P 221391-58-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (synthesis and biol. activity of aryloxaluric acid derivs.)

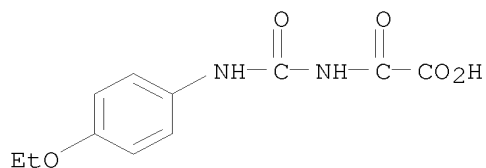
RN 221391-56-6 CAPLUS

CN Acetic acid, 2-oxo-2-[[ (phenylamino)carbonyl]amino]- (CA INDEX NAME)



RN 221391-58-8 CAPLUS

CN Acetic acid, 2-[[[(4-ethoxyphenyl)amino]carbonyl]amino]-2-oxo- (CA INDEX NAME)



IT 221391-60-2P 221391-61-3P 221391-63-5P

221391-65-7P 221391-67-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. activity of aryloxaluric acid derivs.)

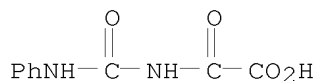
RN 221391-60-2 CAPLUS

CN Acetic acid, 2-oxo-2-[[[(phenylamino)carbonyl]amino]-, compd. with 2-methyl-2-propanamine (1:1) (CA INDEX NAME)

CM 1

CRN 221391-56-6

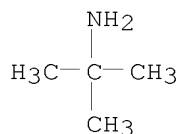
CMF C9 H8 N2 O4



CM 2

CRN 75-64-9

CMF C4 H11 N



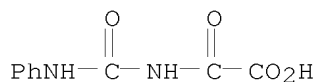
RN 221391-61-3 CAPLUS

CN Acetic acid, 2-oxo-2-[[[(phenylamino)carbonyl]amino]-, compd. with tricyclo[3.3.1.1.3,7]decan-1-amine (1:1) (CA INDEX NAME)

CM 1

CRN 221391-56-6

CMF C9 H8 N2 O4



CM 2

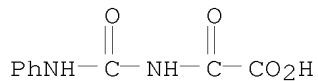
CRN 768-94-5  
CMF C10 H17 N



RN 221391-63-5 CAPLUS  
CN D-Glucose, 2-amino-2-deoxy-, oxo[[ (phenylamino)carbonyl]amino]acetate  
(9CI) (CA INDEX NAME)

CM 1

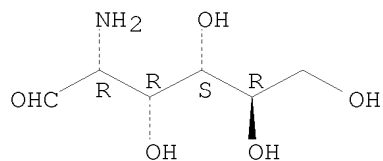
CRN 221391-56-6  
CMF C9 H8 N2 O4



CM 2

CRN 3416-24-8  
CMF C6 H13 N O5

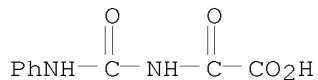
Absolute stereochemistry. Rotation (+).



RN 221391-65-7 CAPLUS  
CN Acetic acid, 2-oxo-2-[[ (phenylamino)carbonyl]amino]-, compd. with  
7-ethoxy-3,9-acridinediamine (1:1) (CA INDEX NAME)

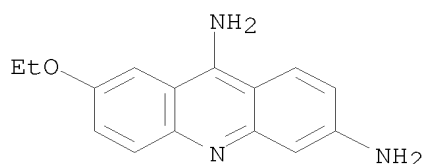
CM 1

CRN 221391-56-6  
CMF C9 H8 N2 O4



CM 2

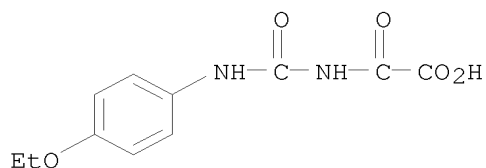
CRN 442-16-0  
CMF C15 H15 N3 O



RN 221391-67-9 CAPLUS  
 CN Acetic acid, 2-[[[(4-ethoxyphenyl)amino]carbonyl]amino]-2-oxo-, compd. with 3,6-acridinediamine (1:1) (CA INDEX NAME)

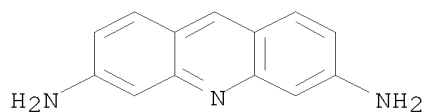
CM 1

CRN 221391-58-8  
 CMF C11 H12 N2 O5

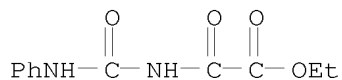


CM 2

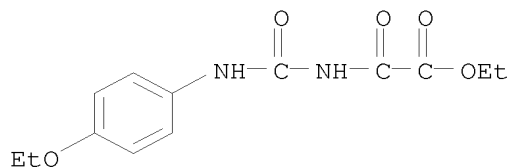
CRN 92-62-6  
 CMF C13 H11 N3



IT 221391-80-6 221391-81-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis and biol. activity of aryloxaluric acid derivs.)  
 RN 221391-80-6 CAPLUS  
 CN Acetic acid, oxo[[ (phenylamino)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 221391-81-7 CAPLUS  
 CN Acetic acid, 2-[[[(4-ethoxyphenyl)amino]carbonyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)





L6 ANSWER 3 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:182339 CAPLUS

DOCUMENT NUMBER: 106:182339

ORIGINAL REFERENCE NO.: 106:29505a,29508a

TITLE: Effect of the initial concentration of organic compounds in water on the results of ozonation  
AUTHOR(S): Gauducheau, Christine; Gilbert, Ernst; Eberle, Siegfried H.

CORPORATE SOURCE: Inst. Radiochem., Kernforschungszent. Karlsruhe, Karlsruhe, D-7500, Fed. Rep. Ger.

SOURCE: Zeitschrift fuer Wasser- und Abwasser-Forschung (1987), 20(1), 6-12  
CODEN: ZWABAQ; ISSN: 0044-3727

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 106:182339

AB To apply the results of ozonization of organic compds. at high concns. (>100 mg/L) to low concns. found in raw water for drinking water treatment, the ozonization of isobarbituric acid (I) [496-76-4] at an initial concentration of

10-3M and 10-5M was investigated at pH values of 3, 7, and 12. At a pH of 3, the ozonization of I (10-3M) leads to the formation of formyloxaluric acid [106055-61-2] and oxaluric acid [585-05-7], and addnl. at pH 7 to HCO<sub>2</sub>H [64-18-6]. At the initial concentration of 10-5M (pH 7)

besides oxaluric acid and HCO<sub>2</sub>H, oxalic acid [144-62-7] and alloxanic acid [470-44-0] are formed. Using the C balance, it is shown that >90% of the organic oxidation products are identified. The results of the ozonization of I at a pH of 12 as well as of the ozonization in the presence of humic acid at a pH of 7 and the reaction of Fenton's reagent show that 2 reaction mechanisms - the direct attack of O<sub>3</sub> or the reaction of the hydroxyl radical - are responsible for the different oxidation products at different conditions. The reaction mechanisms are discussed.

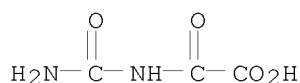
IT 585-05-7P 106055-61-2P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in ozonization of water containing organic compds., concentration and pH effect on)

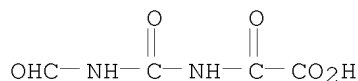
RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



RN 106055-61-2 CAPLUS

CN Acetic acid, 2-[[[(formylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 4 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:38128 CAPLUS

DOCUMENT NUMBER: 106:38128

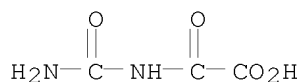
ORIGINAL REFERENCE NO.: 106:6297a

TITLE: Are the results of ozonation of model compounds at high concentrations transferable to the conditions of drinking water treatment with ozone?

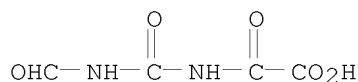
AUTHOR(S): Gauducheau, C.; Gilbert, E.; Eberle, S. H.

CORPORATE SOURCE: Kernforschungszent. Karlsruhe, Karlsruhe, 7500, Fed.

Rep. Ger.  
 SOURCE: Ozone: Science & Engineering (1986), 8(3), 199-216  
 CODEN: OZSEDS; ISSN: 0191-9512  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Ozonization of water containing 10<sup>-3</sup>-10<sup>-5</sup>M concns. of isobarbituric acid (I) [496-76-4], citraconic acid (II) [498-23-7], or o-chlorophenol (III) [95-57-8] at an O<sub>3</sub> dose of 0.1-10 mg/L-min and a pH of 7 resulted in the formation of formyloxaluric acid [106055-61-2], oxaluric acid (V) [585-05-7], and HCOOH (VI) [64-18-6] in the case of I. At an initial concentration of 10<sup>-5</sup>M I/L, alloxanic acid [470-44-0] and oxalic acid (VII) [144-62-7] were formed in addition to V and VI. The oxidation products of II ozonization at 10<sup>-3</sup>M were glyoxylic acid [298-12-4], VI, VII, pyruvic acid [127-17-3], and hydroxypyruvic acid [1113-60-6]. The rate of oxidation of II at a concentration of 10<sup>-5</sup>M was 0.5 of the rate at 10<sup>-3</sup>M. Contrary to the results obtained at 10<sup>-3</sup>M, only 70% of the initial compds. were destroyed after a long ozonization period at an initial concentration of 10<sup>-5</sup>M II. The oxidation rate of III at a concentration of 10<sup>-5</sup>M was twice as fast as at an initial concentration of 10<sup>-3</sup>M; and in both cases yellow compds. were formed. The results of the ozonization of water containing high concns. of compds. at a pH of 7 can be used to qual. predict the oxidation products of an organic pollutant formed after the ozonization of a drinking water and take into account the attack of (OH). radicals at higher pH values.  
 IT 585-05-7P, Oxaluric acid  
 RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in ozonization of drinking water containing isobarbituric acid)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



IT 106055-61-2P  
 RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in ozonization of drinking water containing isobarbituric acid and citraconic acid)  
 RN 106055-61-2 CAPLUS  
 CN Acetic acid, 2-[[[(formylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 5 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1973:466301 CAPLUS  
 DOCUMENT NUMBER: 79:66301  
 ORIGINAL REFERENCE NO.: 79:10715a,10718a  
 TITLE: Quinazolines. I. Oxidation of indole-1,2-dicarboximides and subsequent conversion of their oxidation products to quinazolinones  
 AUTHOR(S): Ishizumi, Kikuo; Inaba, Shigeho; Yamamoto, Hisao  
 CORPORATE SOURCE: Pharm. Div., Sumitomo Chem. Co., Ltd., Takarazuka, Japan

SOURCE: Journal of Organic Chemistry (1973), 38(15),  
2617-9  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 79:66301

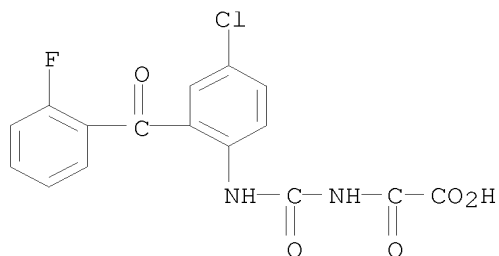
GI For diagram(s), see printed CA Issue.

AB Chromic acid oxidation of indole-1,2-dicarboximides (I, R = Cl, R1 = F; R = NO2, R1 = H) gave imidazolidinetriones (II) which on hydrolysis with base gave the corresponding dihydroquinazolinones (III). Ozonolysis of I gave the ozonides (IV). On heating with water, IV were readily converted to III in nearly quantitative yields. The mechanism for this conversion is discussed.

IT 40387-12-0P 40387-13-1P 40387-14-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

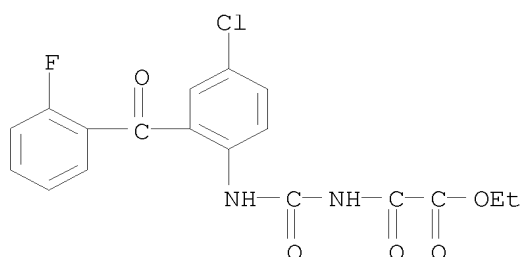
RN 40387-12-0 CAPLUS

CN Acetic acid, [[[[4-chloro-2-(2-fluorobenzoyl)phenyl]amino]carbonyl]amino]oxo- (9CI) (CA INDEX NAME)



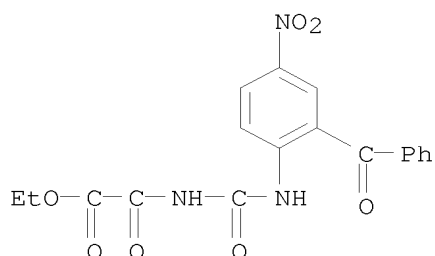
RN 40387-13-1 CAPLUS

CN Acetic acid, [[[[[4-chloro-2-(2-fluorobenzoyl)phenyl]amino]carbonyl]amino]-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)

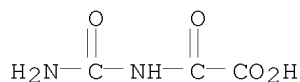


RN 40387-14-2 CAPLUS

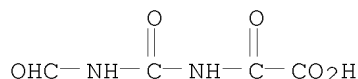
CN Acetic acid, [[[(2-benzoyl-4-nitrophenyl)amino]carbonyl]amino]oxo-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1932:9233 CAPLUS  
 DOCUMENT NUMBER: 26:9233  
 ORIGINAL REFERENCE NO.: 26:1034b-c  
 TITLE: Studies on the physiology of pyrimidines. IV. Further experiments on the intermediary metabolism of uracil  
 AUTHOR(S): Cerecedo, Leopold R.; Curry, Ethel F.; Stekol, Jakob A.; Elbaum, Henry  
 SOURCE: Journal of Biological Chemistry (1931), 93, 269-74  
 CODEN: JBCHA3; ISSN: 0021-9258  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. C. A. 25, 335. Oxaltiric acid, I, and formyloxaluric acid, II, when fed to dogs, were metabolized to urea to the extent of 30-50%. On injection of I subcutaneously similar results were obtained, but II was toxic. The formation of I as an intermediate compound in the metabolism of uracil is therefore postulated.  
 IT 585-05-7, Oxaluric acid 106055-61-2, Oxamic acid, N-formylcarbamyloxy- (metabolism of)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



RN 106055-61-2 CAPLUS  
 CN Acetic acid, 2-[[[(formylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



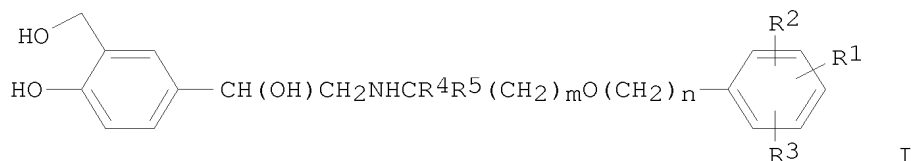
L6 ANSWER 7 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:696862 CAPLUS  
 DOCUMENT NUMBER: 139:230460  
 TITLE: Preparation of phenethanolamines as  $\beta$ 2-adrenoreceptor agonists for treatment of respiratory diseases  
 INVENTOR(S): Blake, Keith; Coe, Diane Mary; Procopiou, Panayiotis Alexandrou  
 PATENT ASSIGNEE(S): Glaxo Group Limited, UK  
 SOURCE: PCT Int. Appl., 99 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072539	A1	20030904	WO 2003-EP2301	20030227 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003210428 A1 20030909 AU 2003-210428 20030227 <--  
EP 1478620 A1 20041124 EP 2003-742975 20030227  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK  
JP 2005519083 T 20050630 JP 2003-571245 20030227  
US 20050209338 A1 20050922 US 2004-506173 20040827  
US 20070249630 A1 20071025 US 2007-766879 20070622  
PRIORITY APPLN. INFO.: GB 2002-4719 A 20020228  
WO 2003-EP2301 W 20030227  
US 2004-506173 B1 20040827

OTHER SOURCE(S): MARPAT 139:230460  
GI

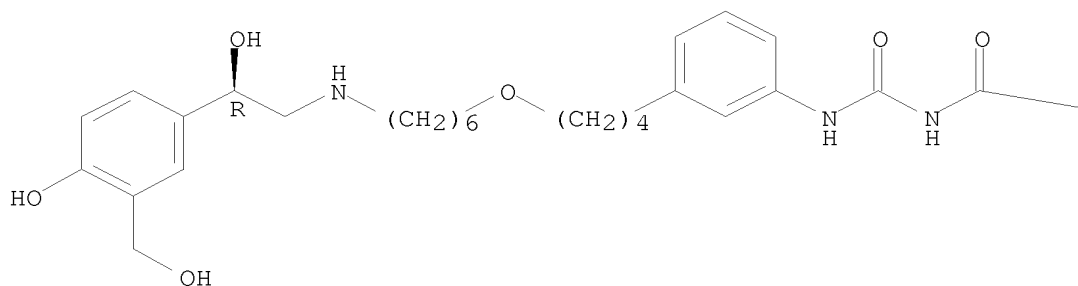


AB The present invention relates to phenethanolamines (shown as I; variables defined below; e.g. N-(4-fluorophenyl)-N'-[3-[4-[6-[[ (2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]hexyl]oxy]butyl]phenyl]urea acetate), to a process for their manufacture, to pharmaceutical compns. containing them, and to their use in therapy, in particular their use in the prophylaxis and treatment of respiratory diseases. At the human beta 2 adrenoreceptor, 37 examples of I had agonist IC50 values <1 μM. For I: m = 2-8; n = 3-11; with the proviso that m + n = 5-19; R1 is -XNR6C(O)NR7R8; wherein X = -(CH2)p- and C2-6alkenylene; R6 and R8 = H, C1-6alkyl and C3-7cycloalkyl; R7 = H, C1-6alkyl, C3-7cycloalkyl, -C(O)R9, Ph, naphthyl, hetaryl, and phenyl(C1-4alkyl)- and R7 is (un)substituted by 1 or 2 halo, hydroxy, C1-6alkyl, C1-6haloalkyl, C1-6alkoxy, -NHC(O)(C1-6alkyl), -SO2(C1-6alkyl), -SO2(phenyl), -CO2H, -CO2(C1-4alkyl) and CONR10R11; p = 0-6. Or R1 is cyclized such that R8 forms a bond with the Ph ring to which R1 is attached, via the ring C atom adjacent to R1, so as to form -NR6C(O)NR7-; R2 = H, C1-6alkyl, C1-6alkoxy, Ph, halo, and C1-6haloalkyl; R3 = H, hydroxy, C1-6alkyl, halo, C1-6alkoxy, Ph, C1-6haloalkyl, and -SO2NR12R13; addnl. details including provisos are given in the claims. Forty-two example preps. of I are included. For example, 1-(4-fluorophenyl)-3-[3-[4-[6-[[ (2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]hexyl]oxy]butyl]phenyl]urea acetate was prepared in 11 steps starting from 2-bromo-1-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)ethanone, Cs2CO3, and di-tert-Bu iminodicarboxylate and involving the following intermediates: di(tert-butyl) 2-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-2-oxoethylimidodicarbonate, tert-Bu [2-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-2-oxoethyl]carbamate, tert-Bu [(2R)-2-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-2-hydroxyethyl]carbamate, (5R)-5-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-1,3-oxazolidin-2-one, 6-bromohexyl 3-butynyl ether, (5R)-3-[6-(but-3-ynyloxy)hexyl]-5-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-1,3-oxazolidin-2-one, (5R)-3-[6-[4-(3-aminophenyl)-3-butynyl]oxy]hexyl]-5-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-1,3-oxazolidin-2-one, (5R)-3-[6-[4-(3-aminophenyl)butoxy]hexyl]-5-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-1,3-oxazolidin-2-one, 1-[3-[4-[6-[(5R)-5-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-2-oxo-1,3-oxazolidin-3-yl]hexyl]oxy]butyl]phenyl]-3-(4-fluorophenyl)urea and 1-[3-[4-[6-[[ (2R)-2-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-2-hydroxyethyl]amino]hexyl]oxy]butyl]phenyl]-3-(4-fluorophenyl)urea.

IT 594862-40-5P, [[[[[3-[4-[[6-[[ (2R)-2-Hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]hexyl]oxy]butyl]phenyl]amino]carbonyl]amino](oxo)acetic acid  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (drug candidate; preparation of phenethanolamines as  $\beta$ 2-adrenoreceptor agonists for treatment of respiratory diseases)  
 RN 594862-40-5 CAPLUS  
 CN Acetic acid, 2-[[[[[3-[4-[[6-[[ (2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]hexyl]oxy]butyl]phenyl]amino]carbonyl]amino]-2-oxo- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



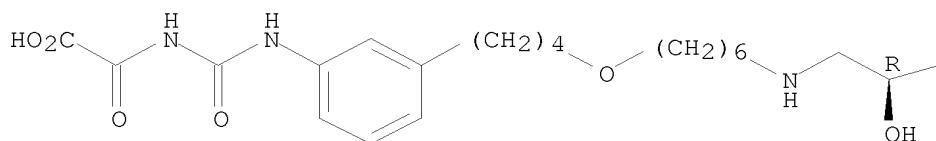
PAGE 1-B

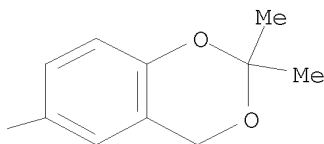
—CO<sub>2</sub>H

IT 594862-44-9P, [[[[[3-[4-[[6-[[ (2R)-2-(2,2-Dimethyl-4H-1,3-benzodioxin-6-yl)-2-hydroxyethyl]amino]hexyl]oxy]butyl]phenyl]amino]carbonyl]amino](oxo)acetic acid  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of phenethanolamines as  $\beta$ 2-adrenoreceptor agonists for treatment of respiratory diseases)  
 RN 594862-44-9 CAPLUS  
 CN Acetic acid, 2-[[[[[3-[4-[[6-[[ (2R)-2-(2,2-dimethyl-4H-1,3-benzodioxin-6-yl)-2-hydroxyethyl]amino]hexyl]oxy]butyl]phenyl]amino]carbonyl]amino]-2-oxo- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



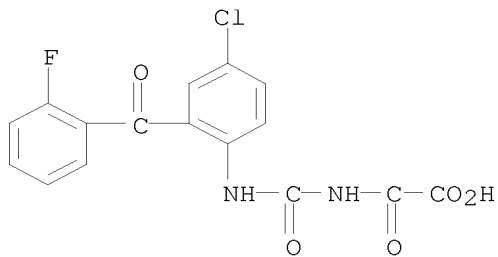


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

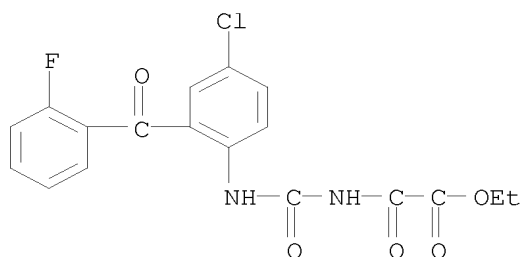
L6 ANSWER 8 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1975:410139 CAPLUS  
 DOCUMENT NUMBER: 83:10139  
 ORIGINAL REFERENCE NO.: 83:1705a,1708a  
 TITLE: Quinazolinone compounds  
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan  
 SOURCE: Neth. Appl., 16 pp.  
 CODEN: NAXXAN  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Dutch  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 7304967	A	19741014	NL 1973-4967	19730410 <--
			NL 1973-4967	A 19730410

PRIORITY APPLN. INFO.:  
 GI For diagram(s), see printed CA Issue.  
 AB Antiinflammatory and analgesic (no date) quinazolinones I(R = Me, R1 = H, R2 = Cl; R = H, R1 = F, R2 = Cl; R = R1 = H, R2 = NO2) were prepared Thus 1-methyl-3-phenyl-5-chloro-2-indolecarbonyl azide was treated with EtOH and the Et carbamate oxidized to 2,4-Bz(Cl)C6H3NMeCONHCO2Et, which on basic hydrolysis gave I(R = Me, R1 = H, R2 = Cl).  
 IT 40387-12-0P 40387-13-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and hydrolysis of)  
 RN 40387-12-0 CAPLUS  
 CN Acetic acid, [[[[4-chloro-2-(2-fluorobenzoyl)phenyl]amino]carbonyl]amino]oxo- (9CI) (CA INDEX NAME)



RN 40387-13-1 CAPLUS  
 CN Acetic acid, [[[[4-chloro-2-(2-fluorobenzoyl)phenyl]amino]carbonyl]amino]-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 9 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:73020 CAPLUS

DOCUMENT NUMBER: 82:73020

ORIGINAL REFERENCE NO.: 82:11675a,11678a

TITLE: Quinazolinone compounds

INVENTOR(S): Ishizumi, Kikuo; Mori, Kazuo; Yamamoto, Michihiro;  
Yamamoto, Hisao; Koshiba, Masao; Inaba, Shigeo

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd.

SOURCE: Can., 25 pp.

CODEN: CAXXA4

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 949573	A1	19740618	CA 1973-168918	19730417 <--
PRIORITY APPLN. INFO.:			CA 1973-168918	A 19730417

OTHER SOURCE(S): MARPAT 82:73020

GI For diagram(s), see printed CA Issue.

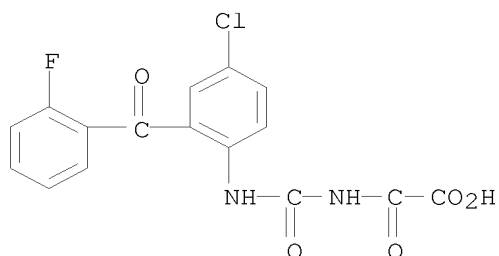
AB The quinazolinones I (R = Me, R1 = H, R2 = Cl; R = H, R1 = F, R2 = Cl; R = R1 = H, R2 = NO2) were prepared by several methods. Thus, 1-methyl-3-phenyl-5-chloroindole-2-carboxylic azide was heated and then treated with PhCH2OH and the resulting carbamate oxidized with chromic anhydride to give 4,2-Cl(PhCO)C6H3NMeCONHCO2CH2Ph, which was cyclized with HCl to give I (R = Me, R1 = H, R2 = Cl).

IT 40387-12-0P 40387-13-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

RN 40387-12-0 CAPLUS

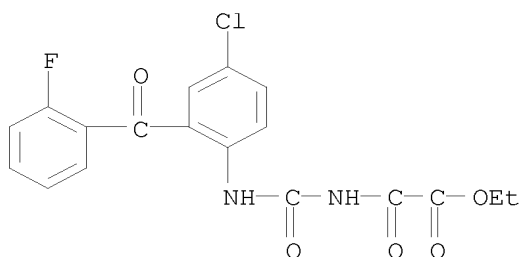
CN Acetic acid, [[[[4-chloro-2-(2-fluorobenzoyl)phenyl]amino]carbonyl]amino]oxo- (9CI) (CA INDEX NAME)



RN 40387-13-1 CAPLUS

CN Acetic acid, [[[[4-chloro-2-(2-fluorobenzoyl)phenyl]amino]carbonyl]amino]-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)





L6 ANSWER 10 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:569016 CAPLUS

DOCUMENT NUMBER: 137:256858

TITLE: Flexible Square Supramolecular Rings with Hydrogen-Bonded Bushing in Solid-State Oxalurate Complexes: Versatility of the Oxalurate Ligand in Covalent and Noncovalent Binding

AUTHOR(S): Falvello, Larry R.; Garde, Raquel; Tomas, Milagros

CORPORATE SOURCE: Department of Inorganic Chemistry and Aragon Materials Science Institute, University of Zaragoza-CSIC, Zaragoza, E-50009, Spain

SOURCE: Inorganic Chemistry (2002), 41(17), 4599-4604

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:256858

AB Isotopic pseudooctahedral complexes of Co, Ni, and Cu with two chelating oxalurate ligands and two H<sub>2</sub>O mols., trans-[M(oxalurate)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>], were synthesized and isolated by a novel progressive crystallization technique. Diffraction analyses reveal that the three complexes form isotopic solid-state structures in which the mol. connectivity and complex network of noncovalent interactions are qual. identical throughout the series. The oxalurate groups form unbounded chains through two different self-recognition patterns—a typical DA-AD motif and an unusual DDA'-A'DD form (D = H bond donor, A' = double acceptor). The unsym. oxalurate group possesses the topol. properties necessary to form aggregates of higher symmetry, and the M(oxalurate)<sub>2</sub> fragments form a rhombic 2-dimensional motif with H-bonded corners and with H-bond acceptors directed to the inside of the cyclic aggregate. The 2-dimensional net is stacked to form a channeled 3-dimensional structure, in which the coordinated aqua ligands form the principal interlayer interactions. The slanted channels are occupied by the axial waters and by waters of crystallization, which are H bonded

to the channel walls to form an ordered bushing. The extensive 3-dimensional H-bonded superstructure is flexible enough to accommodate the distortion produced by the Jahn-Teller effect in the Cu compound without requiring a qual. structural change. The bonds affected by Jahn-Teller distortion in the Cu complex [Cu-O = 2.3788(15) Å] are significantly longer than their analogs in the Co and Ni complexes [Co-O = 2.175(2), Ni-O = 2.094(9) Å].

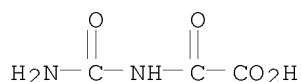
IT 460049-76-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and complexation with transition metals)

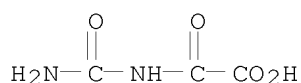
RN 460049-76-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo-, sodium salt (1:1) (CA INDEX NAME)



● Na

IT 585-05-7, Oxaluric acid  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant for preparation of sodium oxalurate)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:639384 CAPLUS

DOCUMENT NUMBER: 117:239384

ORIGINAL REFERENCE NO.: 117:41289a,41292a

TITLE: Ozonation of pyrimidines in aqueous solutions

AUTHOR(S): Gilbert, E.; Hoffmann-Glewe, S.

CORPORATE SOURCE: Inst. Radiochem., Kernforschungszent. Karlsruhe, Karlsruhe, 7500, Germany

SOURCE: Water Research (1992), 26(11), 1533-40

CODEN: WATRAG; ISSN: 0043-1354

DOCUMENT TYPE: Journal

LANGUAGE: English

AB It was demonstrated in all cases that the oxidative attack takes place on C5 or C6 while, depending on the pH, stable 6-ring compds., such as alloxan, 5-ring compds., such as parabanic acid and alloxanic acid, and ring-opening products, such as formyloxaluric acid, oxaluric acid and formic acid are formed. In some cases, H<sub>2</sub>O<sub>2</sub> was detected as the inorg. product. The oxidation of hydantoin causes a quant. production of parabanic acid in acid solution, whereas at pH 7 ring-opening takes place and oxaluric acid was detected as the product of oxidation. From the C balances, >90% of the products were detected.

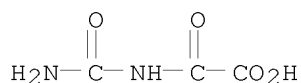
IT 585-05-7P, Oxaluric acid 106055-61-2P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in pyrimidine ozonization, pH effect on, in aqueous solution, water purification in relation to)

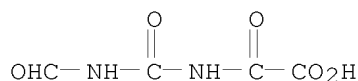
RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



RN 106055-61-2 CAPLUS

CN Acetic acid, 2-[[[(formylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 12 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:75960 CAPLUS

DOCUMENT NUMBER: 66:75960

ORIGINAL REFERENCE NO.: 66:14247a,14250a

TITLE: Synthesis of semioxamazones, semioxamides and their derivatives

AUTHOR(S): Moshchitskii, S. D.; Sologub, L. S.; Pavlenko, A. F.; Akkerman, V. P.

SOURCE: Zhurnal Organicheskoi Khimii (1966), 2(12), 2164-7

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The title compds. R:NCOCONHR1 (I) were prepared by condensation of 5-( $\alpha$ -hydroxy- $\beta,\beta,\beta$ -trichloroethyl)-semioxamazide (II) or of 5-(1H-1,2,4-triazol-3-yl)semioxamazide (III) with a carbonyl compound. Yields of alkyl oxamates were also improved. A solution of 0.1 mole

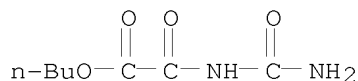
H2NCONH2 in 100 ml. Me2CO was refluxed with addition of 0.12 mole BuO2CCOCl in 20 moles Me2CO 1.5 hrs. Crystallization from the reaction mixture gave N-(butyloxalyl)urea, m. 170-1°, in 80% yield. Similarly, the following RCOCONHR (IV) were prepared (R, R1, m.p., and yield given Et, 1H-1, 2,4-triazolyl, 230-2°, 92; iso-Pr, CH(OH)CCl3, 112-14°, 85; iso-Bu, CONH2, 162-4°, 78. An alc. solution of IV [R = iso-Pr, R1 = CH(OH)CCl3] and N2H4 kept 12 hrs. gave directly II, m. 180-1°, in 60% yield. Similarly, III, m. >300° was obtained in 90% yield. II in a little water heated with cyclopentanone 4 hrs. gave on cooling a precipitate of I [R = cyclopentyl, R1 = CH(OH)CCl3], m. 175-6°, in 80% yield. Similarly, the following I were prepared (R, R1, and m.p. given) CHCCl:CClCO2H, H, 217-18°; cyclopentylidene, H, 163-4°; MeCCO2H, CH2CH2OH, 158-60°; Me2C, CH2CH2OH, 130-1°; CHCCl:CClCO2H, CH2CH2OH, 187-8°; MeCEt, CH2CH2OH, 9 2-3°; p-BrC6H4CH, H, >300°; p-O2NC6H4CH, H, 272-4°; cyclopentylidene, 1H-1,2,4-triazolyl, >300°; cyclopentylidene, CH2CH2OH, 135-6°; isatinyldene, H, >300°; PhCH, 1H-1,2,4-triazolyl, >300°; p-BrC6H4CH, CH2CH2OH, 269-70°; PhCH, CH2CH2OH, 223-5°; PhCMe, 1H-1,2,4-triazolyl, >300°; PhCH, H, 215-16°; PhCMe, CH2CH2OH, 168-70°.

IT 13581-63-0P 13581-65-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

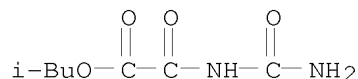
RN 13581-63-0 CAPLUS

CN Oxaluric acid, butyl ester (8CI) (CA INDEX NAME)



RN 13581-65-2 CAPLUS

CN Oxaluric acid, isobutyl ester (8CI) (CA INDEX NAME)



L6 ANSWER 13 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

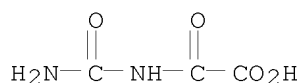
ACCESSION NUMBER: 1966:474751 CAPLUS  
DOCUMENT NUMBER: 65:74751  
ORIGINAL REFERENCE NO.: 65:13997g-h,13998a  
TITLE: Oxidation of guanine and guanosine by bromine  
AUTHOR(S): Shapiro, Robert; Agarwal, Satish C.  
CORPORATE SOURCE: New York Univ., New York, NY  
SOURCE: Biochemical and Biophysical Research Communications ( 1966), 24(3), 401-5  
CODEN: BBRCA9; ISSN: 0006-291X  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB In order to establish the chemical basis for the mutagenic effect of brominating agents, guanine (I) and guanosine (II) were subjected to the action of Br, and the reaction products were investigated. Treatment of I with excess Br in H<sub>2</sub>O at room temperature for several days afforded 38% oxalylguanidine (III), m. >300°. Alternate routes to III were: (1) CrO<sub>3</sub> oxidation of 2-amino-4,6-dihydroxypyrimidine, or (2) condensation of EtO<sub>2</sub>CCO<sub>2</sub>Et with H<sub>2</sub>NC(NH<sub>2</sub>): NH.H<sub>2</sub>CO<sub>3</sub>. The latter reaction also yielded oxalylbiguanide (IV), m. 232-4°. In addition to III, the following degradation products were formed from I upon reaction with Br (method of isolation and percent yield given): oxaluric acid (NH<sub>4</sub><sup>+</sup> salt, 32); guanidine (picrate, 26); and oxalic acid (Ca<sup>++</sup> salt, 24). The presence of urea was also demonstrated chromatographically and estimated spectrophotometrically. Reaction of I with Br in a limited amount of H<sub>2</sub>O gave rise to 8-bromoguanine, from which the same degradation products were produced upon further treatment with aqueous Br. When II was allowed to react with excess Br in H<sub>2</sub>O the initial product (65% yield) was identified as 8-bromoguanosine (V). Upon further reaction, V was degraded to the following products: oxalic acid, guanidine, urea, ribose, D-ribosylurea, and D-ribosyloxaluric acid. Paper chromatography and electrophoresis were used for the separation and identification of these products. The mutagenic action of Br is attributed to destruction of the guanine residues in nucleic acids. The loss of guanine would result in disruption of H bonds and a weakening of the secondary structure of the nucleic acid chains.

IT 13188-21-1  
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 13188-21-1 CAPLUS

CN Oxaluric acid, monoammonium salt (8CI) (CA INDEX NAME)



● NH<sub>3</sub>

(from guanine bromination)

L6 ANSWER 14 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1914:8483 CAPLUS  
DOCUMENT NUMBER: 8:8483  
ORIGINAL REFERENCE NO.: 8:1271g-i  
TITLE: Synthesis of amino-oxalylbiuret, NH<sub>2</sub>COCONHCONHCONH<sub>2</sub>  
AUTHOR(S): Born-Water, J. Th.  
SOURCE: Verslag van de Gewone Vergadering van de Afdeling Natuurkunde, Koninklijke Nederlandse Akademie van Wetenschappen (1914), 22, 190-2  
CODEN: KNWNAC; ISSN: 0368-6329  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB Amido-oxalylbiurel was synthesized in order to prove that it is not

identical with oxalyldiureide. 2 mols. of H<sub>2</sub>NCOCO<sub>2</sub>Et + 1 mol. (COCl)<sub>2</sub> b. in dry C<sub>6</sub>H<sub>6</sub> liberate HCl and on cooling carbonyldi(oxamethane), CO(NHCOCO<sub>2</sub>Et)<sub>2</sub>. seps.; needles, m. 115-6°. (COCl)<sub>2</sub> + mol. amts. of urethan and oxamethane b. in dry C<sub>6</sub>H<sub>6</sub> give α-carbethoxyyl-β-oxalylethoxyluera (a), EtO<sub>2</sub>C CONHCONHCO<sub>2</sub>Et, recrystd. from EtAc, m. 152°. When (a) in EtOH is treated in the cold with dry NH<sub>3</sub> amido-oxalylbiuret seps. as a white amorphous compound, insol. in all usual solvents. The EtOH mother liquor on evaporation gives NH<sub>2</sub>CONHCO<sub>2</sub>Et.

Likewise

(a) when acting with NH<sub>3</sub> in warm solution gives NH<sub>2</sub>CONHCO<sub>2</sub>Et and H<sub>2</sub>NCOCO<sub>2</sub>Et. B. considers that Grimaux's "amide of oxalylbiuretic acid" and the synthetic amido-oxalylbiuret are identical.

IT 871901-91-6P, Oxamic acid, N,N'-carbonylbis-, diethyl ester

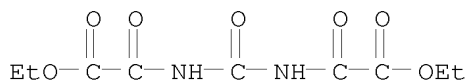
871901-92-7P, Oxamic acid, (carbethoxycarbamyl)-

RL: PREP (Preparation)

(preparation of)

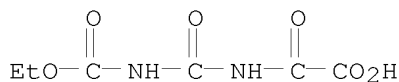
RN 871901-91-6 CAPLUS

CN Oxamic acid, N,N'-carbonylbis-, diethyl ester (1CI) (CA INDEX NAME)



RN 871901-92-7 CAPLUS

CN Acetic acid, 2-[[[(ethoxycarbonyl)amino]carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 15 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1914:8482 CAPLUS

DOCUMENT NUMBER: 8:8482

ORIGINAL REFERENCE NO.: 8:1271g-i

TITLE: Synthesis of amino-oxalylbiuret, NH<sub>2</sub>COCONHCONHCONH<sub>2</sub>

AUTHOR(S): Born-Water, J. Th.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la Belgique (1914), 22, 334-9

CODEN: RTCPB4; ISSN: 0370-7539

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Amido-oxalylbiurel was synthesized in order to prove that it is not identical with oxalyldiureide. 2 mols. of H<sub>2</sub>NCOCO<sub>2</sub>Et + 1 mol. (COCl)<sub>2</sub> b. in dry C<sub>6</sub>H<sub>6</sub> liberate HCl and on cooling carbonyldi(oxamethane), CO(NHCOCO<sub>2</sub>Et)<sub>2</sub>. seps.; needles, m. 115-6°. (COCl)<sub>2</sub> + mol. amts. of urethan and oxamethane b. in dry C<sub>6</sub>H<sub>6</sub> give α-carbethoxyyl-β-oxalylethoxyluera (a), EtO<sub>2</sub>C CONHCONHCO<sub>2</sub>Et, recrystd. from EtAc, m. 152°. When (a) in EtOH is treated in the cold with dry NH<sub>3</sub> amido-oxalylbiuret seps. as a white amorphous compound, insol. in all usual solvents. The EtOH mother liquor on evaporation gives NH<sub>2</sub>CONHCO<sub>2</sub>Et.

Likewise

(a) when acting with NH<sub>3</sub> in warm solution gives NH<sub>2</sub>CONHCO<sub>2</sub>Et and H<sub>2</sub>NCOCO<sub>2</sub>Et. B. considers that Grimaux's "amide of oxalylbiuretic acid" and the synthetic amido-oxalylbiuret are identical.

IT 871901-91-6P, Oxamic acid, N,N'-carbonylbis-, diethyl ester

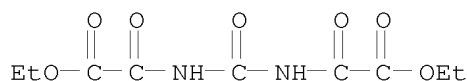
871901-92-7P, Oxamic acid, (carbethoxycarbamyl)-

RL: PREP (Preparation)

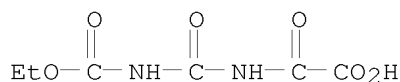
(preparation of)

RN 871901-91-6 CAPLUS

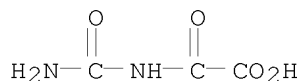
CN Oxamic acid, N,N'-carbonylbis-, diethyl ester (1CI) (CA INDEX NAME)



RN 871901-92-7 CAPLUS  
 CN Acetic acid, 2-[[[(ethoxycarbonyl)amino]carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 16 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1984:1457 CAPLUS  
 DOCUMENT NUMBER: 100:1457  
 ORIGINAL REFERENCE NO.: 100:255a,258a  
 TITLE: Oxalurate induction of multiple URA3 transcripts in *Saccharomyces cerevisiae*  
 AUTHOR(S): Buckholz, Richard G.; Cooper, Terrance G.  
 CORPORATE SOURCE: Dep. Biol. Sci., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA  
 SOURCE: Molecular and Cellular Biology (1983), 3(11), 1889-97  
 CODEN: MCEBD4; ISSN: 0270-7306  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The URA3 gene from *S. cerevisiae* is localized on a 1.1-kilobase (kb) DNA fragment. By using this fragment as a hybridization probe, it was found that oxalurate [585-05-7], a gratuitous inducer of the allantoin degradative system, also serves to induce URA3-specific RNA. This response is restricted to oxalurate; other conditions which bring about high-level synthesis of the allantoin degradative enzymes did not produce the effect. Two classes of RNA (1.0 and 1.5 kb) were found to be oxalurate-induced. Both classes are encoded by the URA3 gene, overlap, and probably do not significantly differ at their 5' termini. Northern blot mapping of the transcripts indicated that the 1.5-kb transcript was likely encoded by sequences extending <0.5 kb downstream from the 3' terminus of the 1.0-kb transcript. Anal. of the endpoints of the major 1.0-kb URA3 transcript by S1 nuclease mapping revealed the existence of two 5' termini, separated by 5-10 nucleotides, and seven 3' termini, separated by 5-20 nucleotides each, over a range of .apprx.70 bases.  
 IT 585-05-7  
 RL: PRP (Properties)  
 (gene URA3 transcription induction by, in *Saccharomyces cerevisiae*)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 17 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:46959 CAPLUS  
 DOCUMENT NUMBER: 132:74531  
 TITLE: Method for knocking out gene transcripts by covalent binding of an antisense probe

INVENTOR(S): Lin, Shi-lung; Ying, Shao-yao  
 PATENT ASSIGNEE(S): Epiclone Inc., USA  
 SOURCE: U.S., 10 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

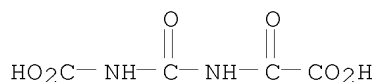
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6015676	A	20000118	US 1998-127368	19980731 <--
WO 2001013959	A1	20010301	WO 1999-US19469	19990826 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9957857	A	20010319	AU 1999-57857	19990826 <--
PRIORITY APPLN. INFO.:			US 1998-127368	A 19980731
			WO 1999-US19469	A 19990826

AB The present invention provides a simple, specific and nontoxic gene knock-out method by formation of covalent bonding between modified probes and targeted sequences. When covalently modified first strand probes are hybridized with a second strand of targeted gene transcripts, certain modified bases of said first strand will interact with natural bases of said second strand to form covalent bonds by which the translation of said second strand is inhibited. Because the hybridization of said two strands generates covalent base-pairing only between their complementary homol. region(s), such specificity increases the targeting efficiency of a gene knock-out system. Also, because neither a polymerase extension reaction nor a nuclease digestion can be performed through the covalently bonded region(s) of aforesaid hybrids, the present invention in conjunction with a delivery method can be used to inactivate intracellular functions of targeted nucleotide sequences, to inhibit viral infections in vivo and to increase binding stability of antisense drugs in a gene therapy.

IT 253801-94-4P  
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)  
 (covalent bond-forming base analog; method for knocking out gene transcripts by covalent binding of an antisense probe)

RN 253801-94-4 CAPLUS

CN Acetic acid, 2-[[[(carboxyamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 18 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:75310 CAPLUS

DOCUMENT NUMBER: 88:75310

ORIGINAL REFERENCE NO.: 88:11895a,11898a

TITLE: Copper phthalocyaninesulfonic acid

INVENTOR(S): Sekiguchi, Tatsuo; Tanaka, Motoo

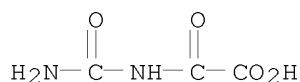
PATENT ASSIGNEE(S): Agency of Industrial Sciences and Technology, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52105933	A	19770906	JP 1976-22762	19760303 <--
JP 54037888	B	19791117		

PRIORITY APPLN. INFO.: JP 1976-22762 A 19760303  
AB Sulfuric acid salts of copper phthalocyanine (I) are heated in the presence of oxalic acid (II) [144-62-7] or II derivs. to give copper phthalocyaninesulfonic acids. Thus, 77 g of I disulfate and 3 g oxalamic acid [471-47-6] were kneaded 30 min at 220-30° and 10 mm, treated in hot aqueous NH<sub>3</sub>, and salted with (NH<sub>4</sub>)<sub>2</sub>CO<sub>3</sub> to give 73 g ammonium copper phthalocyaninedisulfonate [65466-68-4].  
IT 585-05-7  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for sulfonation of copper phthalocyanine)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 19 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

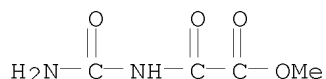
ACCESSION NUMBER: 2003:693525 CAPLUS  
DOCUMENT NUMBER: 139:215960  
TITLE: Waterproof aqueous printing inks containing proton scavengers for high stability, ink cartridges, and ink-jet printers therewith  
INVENTOR(S): Arase, Hidekazu; Soga, Sanemori  
PATENT ASSIGNEE(S): Matsushita Electric Industrial Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003246948	A	20030905	JP 2002-50161	20020226 <--
JP 4015862	B2	20071128		

PRIORITY APPLN. INFO.: JP 2002-50161 20020226  
AB The aqueous inks comprise (A) colorants, (B) moisturizers, (C) water-soluble substances (e.g., hydrolyzable silanes or their partially hydrolyzates) capable of condensation polymerization without water, (D) proton scavengers chosen from carbonyl compds., amides, water-soluble sulfoxides, water-soluble sulfones, hexamethyl phosphoramidate, and cyano compds., and optionally (E) wetting agents. A-C complexes in the inks are stabilized at a wide pH range by the proton scavengers D. Thus, an aqueous ink containing Acid Black 2, glycerin, a reaction product of (MeO)<sub>4</sub>Si and H<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>NH(CH<sub>2</sub>)<sub>2</sub>Si(OMe)<sub>3</sub>, acetone, and diethylene glycol monobutyl ether showed no precipitation at pH 10.5, good discharging from an ink-jet head, and high water resistance when printed.  
IT 530084-26-5  
RL: MOA (Modifier or additive use); TEM (Technical or engineered material

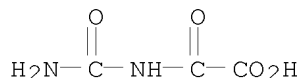


use); USES (Uses)  
 (proton scavengers; aqueous waterproof jet-printing inks containing  
 proton scavengers for high stability)  
 RN 530084-26-5 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo-, methyl ester (CA INDEX  
 NAME)



L6 ANSWER 20 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1963:70892 CAPLUS  
 DOCUMENT NUMBER: 58:70892  
 ORIGINAL REFERENCE NO.: 58:12109e  
 TITLE: Diazotype compositions  
 INVENTOR(S): Schaeffer, Andre  
 PATENT ASSIGNEE(S): Etablissements Bauchet Cie.  
 SOURCE: 17 pp.; Addn. to Fr. 1,249,913 (CA 56, 6831g)  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	FR 78679		19620824	FR 1960-843696	19601110 <--
AB	A mixture of an alkylated or arylated sulfamide and a urea or thiourea is used as the developing agent, and a hydroxycarboxylic acid, an oxamide, a malonamide, a cyanocarboxylic acid, or an oxaluric acid is used as the stabilizing agent.				
IT	585-05-7, Oxaluric acid (derivs. and related compds., as stabilizers in diazotype process)				
RN	585-05-7 CAPLUS				
CN	Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)				



L6 ANSWER 21 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:714471 CAPLUS  
 DOCUMENT NUMBER: 139:359722  
 TITLE: MALDI-TOF mass spectrometry as a powerful tool to study enzymatic processing of DNA lesions inserted into oligonucleotides  
 AUTHOR(S): Gasparutto, D.; Saint-Pierre, C.; Jaquinod, M.; Favier, A.; Cadet, J.  
 CORPORATE SOURCE: Laboratoire des Lesions des Acides Nucleiques, Service Chimie Inorganique Biologique, Grenoble, F-38054, Fr.  
 SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2003), 22(5-8), 1583-1586  
 CODEN: NNNAFY; ISSN: 1525-7770  
 PUBLISHER: Marcel Dekker, Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB MALDI-TOF mass spectrometry measurements, coupled with either exonuclease or DNA N-glycosylases digestions of lesion-containing oligonucleotides, were used to assess biochem. features of several oxidative DNA damage. The latter anal. approach was shown to be an informative and efficient

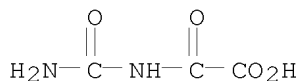
alternative technique to conventional electrophoresis and chromatog. analyses.

IT 585-05-7, Oxaluric acid  
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(MALDI-TOF mass spectrometry as a powerful tool to study enzymic processing of DNA lesions inserted into oligonucleotides)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 22 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:199953 CAPLUS

DOCUMENT NUMBER: 138:409646

TITLE: A computational and experimental search for polymorphs of parabanic acid - a salutary tale leading to the crystal structure of oxo-ureido-acetic acid methyl ester

AUTHOR(S): Lewis, T. C.; Tocher, D. A.; Day, G. M.; Price, S. L.  
CORPORATE SOURCE: Centre for Theoretical and Computational Chemistry, University College London, London, WC1H 0AJ, UK

SOURCE: CrystEngComm (2003), 5, 3-9  
CODEN: CRECF4; ISSN: 1466-8033  
URL: <http://www.rsc.org/CFCart/displayarticleonfree.cfm?article=8%2D9%223%24%5DVZB%214%2E%5FL1%286%2COZ5%2D%40%3CP5H%3D29%23%3C%0A>

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB A computational search to predict the crystal structure of parabanic acid produced the known P21/c/c crystal structure as the global min. in the lattice energy. However, there are many hypothetical structures only 2-6 kJ mol<sup>-1</sup> less stable than the known form, which are within the energy range of possible polymorphism and have reasonable mech. properties and relative growth rates. The harmonic intermol. frequencies and the attachment energy estimate of relative growth rates suggest that the known polymorph is thermodynamically and kinetically favored, but the possibility of other polymorphs cannot be excluded. A simultaneous exptl. search for new polymorphs found crystals with a new morphol. and x-ray powder pattern when a solution of parabanic acid in MeOH was left to evaporate

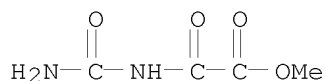
Eventually, the structure was shown by single crystal x-ray diffraction to be that of oxo-ureido-HOAc Me ester (triclinic space group P.hivin.1). Thus, under the conditions of recrystn. from MeOH, parabanic acid had undergone a previously unreported ring-opening reaction, and had not crystallized as a new polymorph as had seemed likely prior to single crystal characterization. The combination of the exptl. and theor. studies indicates that new polymorphs of parabanic acid are unlikely to be found readily.

IT 530084-26-5

RL: PRP (Properties)  
(crystal structure of)

RN 530084-26-5 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 23 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:931417 CAPLUS

DOCUMENT NUMBER: 136:65119

TITLE: Oxidation of 7,8-Dihydro-8-oxoguanine Affords Lesions That Are Potent Sources of Replication Errors in Vivo  
AUTHOR(S): Henderson, Paul T.; Delaney, James C.; Gu, Feng; Tannenbaum, Steven R.; Essigmann, John M.

CORPORATE SOURCE: Division of Bioengineering and Environmental Health and Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Biochemistry (2002), 41(3), 914-921

CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three single-stranded DNA genomes have been constructed that contain the 8-oxo-7,8-dihydro-2'-deoxyguanosine (8-oxodG) oxidation products oxaluric acid, oxazolone, and cyanuric acid. Oligonucleotides containing each lesion were synthesized by treating an oligonucleotide containing a single 8-oxodG with peroxyxynitrite, and the desired products were isolated by HPLC. The modified oligonucleotides were ligated into M13mp7L2 bacteriophage DNA in such a way that the lesion was situated at a known site in the lacZ gene fragment of the viral genome. The circular genomes were transfected into wild-type AB1157 Escherichia coli. The relative efficiency of lesion bypass by DNA polymerase was determined by counting the number of initial independent infections produced by each genome relative to that of an unmodified DNA control. Viral progeny were analyzed for mutation frequency and type by PCR amplification of the insert region followed by a recently developed post-labeling assay. All three secondary lesions were readily bypassed, causing G → T transversions at frequencies at least an order of magnitude higher than 8-oxodG. These data establish a model whereby the modestly mutagenic primary lesion 8-oxodG is oxidized in vivo to much more highly mutagenic secondary lesions.

IT 585-05-7, Oxaluric acid

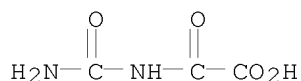
RL: ADV (Adverse effect, including toxicity); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(mutagenic potential of 8-oxo-7,8-dihydro-2'-deoxyguanosine oxidation products oxaluric acid, oxazolone, and cyanuric acid tested by inserting oligonucleotides containing each of these into bacteriophage

DNA and transfection into Escherichia)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 24 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:924460 CAPLUS

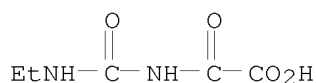
DOCUMENT NUMBER: 136:162488

TITLE: Peroxynitrite Reacts with 8-Nitropurines to Yield 8-Oxopurines

AUTHOR(S): Lee, Joseph M.; Niles, Jacquin C.; Wishnok, John S.;  
Tannenbaum, Steven R.  
CORPORATE SOURCE: Division of Bioengineering and Environmental Health  
and Department of Chemistry, Massachusetts Institute  
of Technology, Cambridge, MA, 02139, USA  
SOURCE: Chemical Research in Toxicology (2002),  
15(1), 7-14  
CODEN: CRTOEC; ISSN: 0893-228X  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Peroxynitrite reacts with 2'-deoxyguanosine to yield several major products, including 8-oxo-2'-deoxyguanosine (8-oxodG) and 8-nitroguanine (8-nitroGua). While the terminal products formed during the reaction of 8-oxodG with peroxynitrite have been previously characterized, those formed from 8-nitroGua have not. To identify these products, 9-ethyl-8-nitroxanthine was used as a model for 8-nitroGua, since the former could be easily synthesized in high yield, and facilitated reversed-phase HPLC separation of the resulting products. Using this model substrate, the products formed during the peroxynitrite reaction were identified as the Et derivs. of oxaluric acid, 5-iminoimidazolidin-2,4-dione, [N-nitro-N'-[2,4-dioxo-imidazolidine-5-ylidene]-urea], dehydroallantoin, parabanic acid, cyanuric acid, and uric acid. Upon the basis of the previous studies with 8-oxodG, these products were recognized as those expected to arise from peroxynitrite-mediated uric acid oxidation. Furthermore, the presence of uric acid in the reaction mixture led us to propose a model in which the 8-nitropurine is first converted to the 8-oxopurine which is further oxidized by peroxynitrite to give the observed final products. We have also provided evidence suggesting that the peroxynitrite anion, acting as a nucleophile, might be responsible for the initial conversion of the 8-nitropurine to the 8-oxopurine and that a hydroxyl radical or oxidative process is less likely to explain this conversion.

IT 105919-00-4  
RL: BSU (Biological study, unclassified); FMU (Formation, unclassified);  
PRP (Properties); BIOL (Biological study); FORM (Formation,  
nonpreparative)  
(peroxynitrite reacts with nitropurines to yield oxopurines)  
RN 105919-00-4 CAPLUS  
CN Acetic acid, 2-[[ (ethylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 25 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:875313 CAPLUS  
DOCUMENT NUMBER: 136:218482  
TITLE: Electrochemically mediated bleaching of pulp fibers  
AUTHOR(S): Kim, H.-C.; Mickel, M.; Bartling, S.; Hampf, N.  
CORPORATE SOURCE: Institute of Physical Chemistry, University of  
Marburg, Marburg, D-35032, Germany  
SOURCE: Electrochimica Acta (2001), 47(5), 799-805  
CODEN: ELCAAV; ISSN: 0013-4686  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

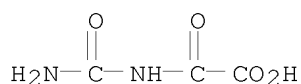
AB Electrochem. delignification is a promising approach for the development of environmentally friendly processes in pulp bleaching. In the process described here, an electrochem. generated organic radical is used to oxidize the lignin selectively. This mol. has low mol. weight and a radical-lifetime

in the tens of minutes range when generated in water at temps. between 50 and 70°. A favorable mediator mol., which is consistent with most of the demands for a tech. process, is violuric acid (I). Delignification of .apprx.35% is obtained with 4 kg/tonpulp. The I mediator is not fully reversible in this process. The mechanism of the degradation of the mediator is still under investigation. The products generated from I during the delignification process are alloxan, parabanic acid, and oxaluric acid. A demonstration setup, which allows studying the possible tech. implementations of this electrochem. process, is described.

IT 585-05-7, Oxaluric acid  
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
 (lignin oxidation by electrochem generated violuric acid radicals for environmental pollution control in pulp bleaching)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 26 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:752001 CAPLUS

DOCUMENT NUMBER: 136:200398

TITLE: Characterization of an oxaluric acid derivative as a guanine oxidation product

AUTHOR(S): Seguy, Christel; Pratviel, Genevieve; Meunier, Bernard

CORPORATE SOURCE: Laboratoire de Chimie de Coordination du CNRS, Toulouse, 31077, Fr.

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (20), 2116-2117  
 CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:200398

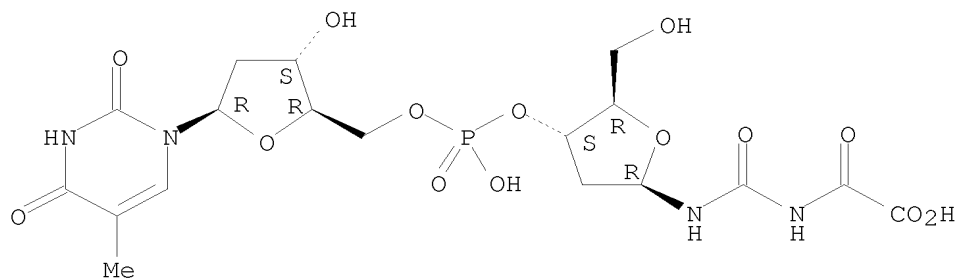
AB The oxidation of guanine in the dinucleoside monophosphate d(GpT) by an oxo-metalloporphyrin generates a linear oxaluric acid derivative after heating at 65 °C for 30 min and at neutral pH.

IT 400781-62-6P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (mol. structure of an oxaluric acid derivative as a guanine oxidation product of dinucleoside monophosphate d(GpT) by an oxo-metalloporphyrin)

RN 400781-62-6 CAPLUS

CN 5'-Thymidylic acid, 5'→3'-ester with [[[2-deoxy-β-D-erythro-pentofuranosyl)amino]carbonyl]amino]oxoacetic acid (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 27 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:508104 CAPLUS

DOCUMENT NUMBER: 135:103250

TITLE: Locating Nucleobase Lesions within DNA Sequences by MALDI-TOF Mass Spectral Analysis of Exonuclease Ladders

AUTHOR(S): Tretyakova, Natalia; Matter, Brock; Ogdie, Alexis; Wishnok, John S.; Tannenbaum, Steven R.

CORPORATE SOURCE: Department of Medicinal Chemistry, University of Minnesota Cancer Center, Minneapolis, MN, 55455, USA

SOURCE: Chemical Research in Toxicology (2001), 14(8), 1058-1070

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The location of carcinogen-modified nucleobases (DNA adducts) within DNA sequences is a critical factor affecting their promutagenic properties and persistence in DNA. We now report the use of controlled exonuclease digestion followed by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) to directly map modified nucleobases within DNA. The DNA sequence is determined by mass spectral anal.

of the DNA ladders produced by sequential removal of nucleotides with either 5'→3' or 3'→5' exonuclease. Individual mononucleotides are identified from the mass differences between adjacent peaks corresponding to singly charged ions of the products of enzymic cleavage. Chemical modified nucleotides are detected and identified by their

mol. weight The resolution and mass accuracy of this approach are sufficient to

identify nucleobase modifications differing in mass by as little as 2 Da. No a priori information on the DNA sequence or adduct type is required. We demonstrate the general applicability of this method by sequencing synthetic oligonucleotides containing a range of nucleobase modifications: O6-methylguanine, peroxyxynitrite-induced oxidative lesions (oxaluric acid, oxazolone, cyanuric acid), and the N2-guanine adduct of (+,-)-7r,8t-dihydroxy-9t,10t-epoxy-7,8,9,10-tetrahydribenzo[a]pyrene. Sequence information is also obtained for DNA oligodeoxynucleotides containing

O6-pyridyloxobutylguanine, despite the ability of this lesion to block 3'-phosphodiesterase.

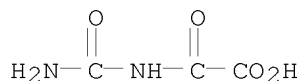
IT 585-05-7P, Oxaluric acid

RL: BOC (Biological occurrence); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(locating nucleobase lesions within DNA sequences by MALDI-TOF mass spectral anal. of exonuclease ladders)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 28 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:84601 CAPLUS

DOCUMENT NUMBER: 134:291401

TITLE: Repair and Mutagenic Potential of Oxaluric Acid, a Major Product of Singlet Oxygen-Mediated Oxidation of 8-Oxo-7,8-dihydroguanine

AUTHOR(S): Duarte, Victor; Gasparutto, Didier; Jaquinod, Michel; Ravanat, Jean-Luc; Cadet, Jean

CORPORATE SOURCE: Laboratoire des Lésions des Acides Nucleiques Service de Chimie Inorganique et Biologique UMR 5046  
Departement de Recherche Fondamentale sur la Matiere Condensee, CEA Grenoble, Grenoble, F-38054, Fr.

SOURCE: Chemical Research in Toxicology (2001), 14(1), 46-53  
CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

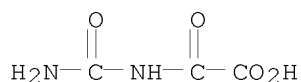
LANGUAGE: English

AB Oxidative reactions within DNA commonly result in base modifications. Among the four DNA bases, guanine is the most susceptible to various oxidants, and its related oxidized form, 8-oxo-7,8-dihydroguanine, has been extensively studied in terms of repair and mutagenicity. However, 8-oxo-7,8-dihydroguanine is readily subjected to further oxidation, and this has become a point of interest. We recently found that singlet oxygen oxidation of 8-oxo-7,8-dihydroguanine led to the predominant formation of oxaluric acid as the final product. We report herein on the biol. features of oxaluric acid dealing with in vitro DNA synthesis and its removal from DNA by repair enzymes. Nucleotide insertion opposite oxaluric acid, catalyzed by Kf exo- and Taq indicates, that oxaluric acid induces G to T and G to C transversions. On the other hand, oxaluric acid represents a block when synthesis is performed with pol  $\beta$ . Interestingly, DNA repair expts. carried out with formamidopyrimidine DNA N-glycosylase (Fpg) and endonuclease III (endo III) show that oxaluric acid is a substrate for both enzymes. Values of  $k_{cat}/K_m$  for the Fpg-mediated removal of oxidative guanine lesions revealed that 8-oxoGua is only a slightly better substrate than oxaluric acid. Interestingly, the results obtained with endo III suggest that oxaluric acid is a much better substrate than is 5-hydroxycytosine (5-OHC), an oxidized pyrimidine base.

IT 585-05-7, Oxaluric Acid  
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
(repair and mutagenic potential of oxaluric acid, major product of singlet oxygen-mediated oxidation of oxodihydroguanine)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 29 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:847281 CAPLUS

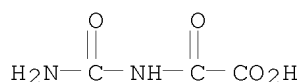
DOCUMENT NUMBER: 134:143403

TITLE: Oxaluric acid as the major product of singlet oxygen-mediated oxidation of 8-oxo-7,8-dihydroguanine in DNA

AUTHOR(S): Duarte, Victor; Gasparutto, Didier; Yamaguchi, Lydia F.; Ravanat, Jean-Luc; Martinez, Glaucia R.; Medeiros, Marisa H. G.; Di Mascio, Paolo; Cadet, Jean

CORPORATE SOURCE: Laboratoire des Lésions des Acides Nucleiques Service de Chimie Inorganique et Biologique Departement de Recherche Fondamentale sur la Matiere Condensee, CEA Grenoble, Grenoble, F-38054, Fr.

SOURCE: Journal of the American Chemical Society (2000), 122(51), 12622-12628  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Oxidative reactions of DNA commonly result in base modifications. Among the 4 DNA bases, guanine is the most susceptible to oxidation, and 1 of its main oxidized compds., namely 8-oxo-7,8-dihydroguanine (I), has been extensively studied in terms of formation, repair, and mutagenicity. However, the latter modified purine base is readily subjected to further oxidation reactions which have recently become a matter of interest. Emphasis was placed in this work on the identification of the final singlet O oxidation products of I in single-stranded DNA. Oxaluric acid was the predominant product of the reaction. Insights in the mechanistic pattern of oxaluric acid formation were gained from isotopic labeling expts. in association with mass spectrometry measurements. Oxaluric acid is formed via an oxidized guanidinohydantoin intermediate, arising from the likely degradation of a transient 5-hydroperoxide. Two subsequent hydrolytic steps that are accompanied by the release of guanidine are likely to be involved in the formation of oxaluric acid.  
 IT 585-05-7P, Oxaluric acid  
 RL: BSU (Biological study, unclassified); MFM (Metabolic formation); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)  
 (oxaluric acid as the major product of singlet oxygen-mediated oxidation of 8-oxo-7,8-dihydroguanine in DNA)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

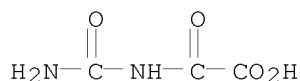
L6 ANSWER 30 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:734086 CAPLUS  
 DOCUMENT NUMBER: 134:247861  
 TITLE: Roles of the Dal82p domains in allophanate/oxalurate-dependent gene expression in Saccharomyces cerevisiae  
 AUTHOR(S): Scott, Stephanie; Abul-Hamd, Ashraf T.; Cooper, Terrance G.  
 CORPORATE SOURCE: Department of Microbiology and Immunology, University of Tennessee, Memphis, TN, 38163, USA  
 SOURCE: Journal of Biological Chemistry (2000), 275(40), 30886-30893  
 CODEN: JBCHA3; ISSN: 0021-9258  
 PUBLISHER: American Society for Biochemistry and Molecular Biology  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Allophanate/oxalurate-induced gene expression in Saccharomyces cerevisiae requires at least five transcription factors, four of which act pos. (Gln3p, Gat1p, Dal81p, and Dal82p) and one neg. (Dal80p). Gln3p binds to and Gat1p is proposed to bind to single GATA sequences; Dal80p binds to pairs of specifically oriented and spaced GATA sequences, and Dal82p binds to a pathway-specific element, UISALL. Dal82p consists of at least three domains as follows: (i) UISALL DNA-binding, (ii) transcriptional activation, and (iii) coiled-coilDAL82. Here we show that the coiled-coilDAL82 domain possesses two demonstrable functions. (i) It prevents Dal82p-mediated transcription when inducer is absent. (ii) It is



a major, although not exclusive, domain through which the inducer signal is received. Supporting the latter conclusion, a 38-amino acid fragment, containing little more than the coiled-coilDAL82 domain, supports oxalurate-inducible, Dal81p-dependent, reporter gene transcription. Dal81p is required for inducer responsiveness of LexAp-Dal82p and LexAp coiled-coilDAL82-mediated transcription but is not needed for inducer-dependent activation mediated by a Dal82p containing deletions in both the coiled-coilDAL82, UISALL-binding domains. There may be an interaction between Dal81p and the coiled-coilDAL82 domain since (i) Dal81p is required for transcription mediated by LexA-coiled-coilDAL82P and (ii) a Dal81p-Dal82p complex is detected by two-hybrid assay.

IT 585-05-7  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (roles of Dal82p domains in allophanate/oxalurate-dependent gene expression in *Saccharomyces cerevisiae*)

RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 31 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:425918 CAPLUS

DOCUMENT NUMBER: 133:218699

TITLE: Peroxynitrite-Induced Secondary Oxidative Lesions at Guanine Nucleobases: Chemical Stability and Recognition by the Fpg DNA Repair Enzyme

AUTHOR(S): Tretyakova, Natalia Y.; Wishnok, John S.; Tannenbaum, Steven R.

CORPORATE SOURCE: Division of Bioengineering and Environmental Health and Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Chemical Research in Toxicology (2000), 13(7), 658-664

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Synthetic oligodeoxynucleotides containing secondary oxidative lesions at guanine nucleobases have been prepared by the site-specific oxidation by ONOO-

of oligomers containing 8-oxoguanine (8-oxo-G). The oligomers have been tested for their stability to the standard hot piperidine treatment that is commonly used to uncover oxidized DNA lesions. While DNA containing

oxaluric

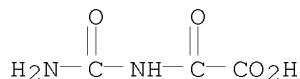
acid and oxazolone was cleaved at the site of modification under hot piperidine conditions, the corresponding cyanuric acid and 8-oxo-G lesions were resistant to piperidine. The recognition of the oxidative lesions by formamidopyrimidine glycosylase (Fpg enzyme) was examined in double-stranded versions of the synthetic oligodeoxynucleotides. Fpg efficiently excised 8-oxo-G and oxaluric acid and to some extent oxazolone, but not cyanuric acid. These data suggest that some DNA lesions formed via ONOO- exposures (cyanuric acid) are not repaired by Fpg and are not uncovered by assays based on piperidine cleavage at the site of lesion. Our results indicate that cryptic secondary and tertiary oxidation products arising from 8-oxo-G may contribute to the overall mutational spectra arising from oxidative stress.

IT 585-05-7, Oxaluric acid

RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent) (DNA lesion; peroxyxynitrite-induced secondary oxidative lesions at guanine nucleobases and chemical stability and recognition by formamidopyrimidine glycosylase DNA repair enzyme)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 32 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:229095 CAPLUS

DOCUMENT NUMBER: 133:43741

TITLE: A Novel Nitration Product Formed during the Reaction of Peroxynitrite with 2',3',5'-Tri-O-acetyl-7,8-dihydro-8-oxoguanosine: N-Nitro-N'-[1-(2,3,5-Tri-O-acetyl-β-D-erythro-pentofuranosyl)-2,4-dioxoimidazolidin-5-ylidene]guanidine

AUTHOR(S): Niles, Jacquin C.; Wishnok, John S.; Tannenbaum, Steven R.

CORPORATE SOURCE: Division of Bioengineering and Environmental Health and Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Chemical Research in Toxicology (2000), 13(5), 390-396

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:43741

AB A novel nitration product, formed during the reaction of peroxyxynitrite with 2',3',5'-tri-O-acetyl-7,8-dihydro-8-oxoguanosine, has been characterized using a combination of UV/vis, CD, and NMR spectroscopy and mass spectrometry. This compound has been identified as N-nitro-N'-[1-(2,3,5-tri-O-acetyl-β-D-erythro-pentofuranosyl)-2,4-dioxoimidazolidin-5-ylidene]guanidine (IV). Upon base hydrolysis, IV releases nitroguanidine (IVa) and an intermediate, 1-(2,3,5-tri-O-acetyl-β-D-erythro-pentofuranosyl)-5-iminoimidazolidine-2,4-dione (IVb). This intermediate is ultimately hydrolyzed to the stable 3-(2,3,5-tri-O-acetyl-β-D-erythro-pentofuranosyl)oxaluric acid (IVc). IV can be reduced by sodium borohydride to a pair of stable diastereomers (IVred). The formation of this product is rationalized in terms of initial oxidation of 2',3',5'-tri-O-acetyl-7,8-dihydro-8-oxoguanosine to a quinonoid diimine intermediate. Combination of this radical species with nitrogen dioxide results in the formation of product IV.

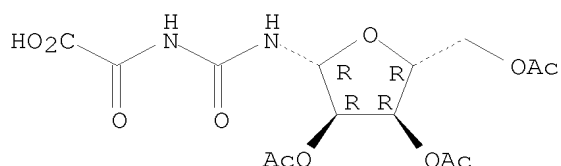
IT 275363-42-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (nitration product formed during the reaction of peroxyxynitrite with dihydrooxoguanosine)

RN 275363-42-3 CAPLUS

CN Acetic acid, oxo[[[(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 33 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:816936 CAPLUS

DOCUMENT NUMBER: 132:229376

TITLE: Photocatalysed degradation of uracil in aqueous titanium dioxide suspensions: mechanisms, pH and cadmium chloride effects

AUTHOR(S): Jaussaud, C.; Paisse, O.; Faure, R.

CORPORATE SOURCE: Laboratoire d'Instrumentation et de Chimie Analytique en Solution (LICAS), Universite Claude Bernard Lyon 1, Villeurbanne, 69622, Fr.

SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (2000), 130(2-3), 157-162

CODEN: JPPCEJ; ISSN: 1010-6030

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Upon UV irradiation, in O2 saturated aqueous titanium dioxide suspensions, uracil is

almost completely mineralized. Most of the organic compds. occurring during the photodegrdn. process have been identified by means of liquid chromatog. and mass spectrometry coupled techniques (LC-MS). The first step of the mineralization leads to the formation of uracilglycol. Then, the main products generated during the photodegrdn. exhibit new functions such as polyol, carboxylic and aldehyde. The presence of urea has been clearly evidenced. At the end of the process, the ultimate step is the formation of nitrate and ammonium ions. The formation kinetics of intermediate products are modified by pH variation and CdCl2 addition

IT 106055-61-2P

RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

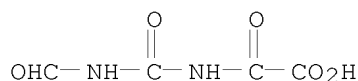
(photoproduct; photocatalyzed degradation of uracil in aqueous titanium

dioxide

suspensions)

RN 106055-61-2 CAPLUS

CN Acetic acid, 2-[[[(formylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 34 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:750890 CAPLUS

DOCUMENT NUMBER: 132:89153

TITLE: Synergistic operation of the CAR2 (ornithine transaminase) promoter elements in Saccharomyces cerevisiae

AUTHOR(S): Park, Heui-Dong; Scott, Stephanie; Rai, Rajendra; Dorrington, Rosemary; Cooper, Terrance G.

CORPORATE SOURCE: Department of Food Science and Technology, Kyungpook National University, Taegu, 702-701, S. Korea

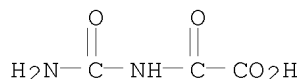
SOURCE: Journal of Bacteriology (1999), 181(22),  
7052-7064  
CODEN: JOBAAY; ISSN: 0021-9193  
PUBLISHER: American Society for Microbiology  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Dal82p binds to the UISALL sites of allophanate-induced genes of the allantoin-degradative pathway and functions synergistically with the GATA family Gln3p and Gat1p transcriptional activators that are responsible for nitrogen catabolite repression-sensitive gene expression. CAR2, which encodes the arginine-degradative enzyme ornithine transaminase, is not nitrogen catabolite repression sensitive, but its expression can be modestly induced by the allantoin pathway inducer. The dominant activators of CAR2 transcription have been thought to be the ArgR and Mcm1 factors, which mediate arginine-dependent induction. These observations prompted the authors' to investigate the structure of the CAR2 promoter with the objectives of determining whether other transcription factors were required for CAR2 expression and, if so, of ascertaining their relative contributions to CAR2's expression and control. The authors show that Rap1p binds upstream of CAR2 and plays a central role in its induced expression irrespectively of whether the inducer is arginine or the allantoin pathway inducer analog oxalurate (OXLU). The data also explain the report that ornithine transaminase production is induced when cells are grown with urea. OXLU induction derives from the Dal82p binding site, which is immediately downstream of the Rap1p site, and Dal82p functions synergistically with Rap1p. This synergism is unlike all other known instances of Dal82p synergism, namely, that with the GATA family transcription activators Gln3p and Gat1p, which occurs only in the presence of an inducer. The observations reported suggest that CAR2 gene expression results from strong constitutive transcriptional activation mediated by Rap1p and Dal82p being balanced by the down regulation of an equally strong transcriptional repressor, Ume6p. This balance is then tipped in the direction of expression by the presence of the inducer. The formal structure of the CAR2 promoter and its operation closely follow the model proposed for CAR1.

IT 585-05-7  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(ornithine transaminase CAR2 gene promoter transcription activation in *Saccharomyces cerevisiae* in response to)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 35 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:684980 CAPLUS

DOCUMENT NUMBER: 132:46092

TITLE: Peroxynitrite reaction products of  
3',5'-di-O-acetyl-8-oxo-7,8-dihydro-2'-deoxyguanosine  
AUTHOR(S): Niles, Jacquin C.; Burney, Samar; Singh, Sukhjeet P.;  
Wishnok, John S.; Tannenbaum, Steven R.

CORPORATE SOURCE: Division of Bioengineering and Environmental Health,  
Massachusetts Institute of Technology, Cambridge, MA,  
02139, USA

SOURCE: Proceedings of the National Academy of Sciences of the  
United States of America (1999), 96(21),  
11729-11734  
CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Of the DNA bases, peroxyxynitrite (ONOO-) is most reactive toward 2'-deoxyguanosine (dGuo), but even more reactive with 8-oxo-7,8-dihydro-2'-deoxyguanosine (8-oxodGuo), requiring a 1,000-fold excess of dGuo to provide 50% protection against the reaction with 8-oxodGuo. Therefore, it seems reasonable that 8-oxodGuo is a potentially important target in DNA and that the structures of the reaction products with ONOO- should be characterized. Using 3',5'-di-O-Ac-8-oxodGuo as a model compound, the reaction products with ONOO- have been isolated and identified under simulated physiol. reaction conditions (phosphate/bicarbonate buffer at pH 7.2). The major reaction product, II, is unstable and undergoes base-mediated hydrolysis to 2,5-diaminoimidazol-4-one, IIa, and 3-(3,5-di-O-Ac-2-deoxy-β-D-erythro-pentofuranosyl)-5-iminoimidazolidine-2,4-dione, IIb. The latter compound further hydrolyzes to 3-(3,5-di-O-Ac-2-deoxy-β-D-erythro-pentofuranosyl)oxaluric acid, IIc. Other products include 3-(3,5-di-O-Ac-2-deoxy-β-D-erythro-pentofuranosyl)-2,4,6-tri oxo-[1,3,5]triazinane-1-carboxamidine, I, which further hydrolyzes to 1-(3,5-di-O-Ac-2-deoxy-β-D-erythro-pentofuranosyl)cyanuric acid, Ia. 1-(3,5-Di-O-Ac-2-deoxy-β-D-erythro-pentofuranosyl)paraban ic acid, III, is a minor product that also may contribute to formation of IIc. The major products formed in these reactions are biol. uncharacterized but are similar to modified DNA bases that have been shown to be both premutagenic and blocks to DNA

polymerization

IT 252743-05-8

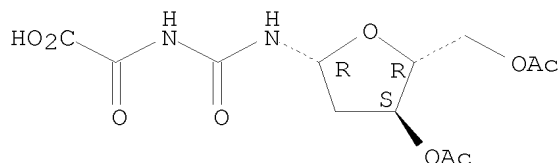
RL: ADV (Adverse effect, including toxicity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(peroxynitrite reaction products of 3',5'-di-O-acetyl-8-oxo-7,8-dihydro-2'-deoxyguanosine in relation to DNA damage)

RN 252743-05-8 CAPLUS

CN Acetic acid, [[[3,5-di-O-acetyl-2-deoxy-β-D-erythro-pentofuranosyl)amino]carbonyl]amino]oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 36 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:313329 CAPLUS

DOCUMENT NUMBER: 131:180989

TITLE: DNA damage in deoxynucleosides and oligonucleotides treated with peroxyxynitrite

AUTHOR(S): Burney, Samar; Niles, Jacquin C.; Dedon, Peter C.; Tannenbaum, Steven R.

CORPORATE SOURCE: Department of Chemistry and Division of Bioengineering and Environmental Health, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Chemical Research in Toxicology (1999), 12(6), 513-520

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Peroxyxynitrite (ONOO-) is a powerful oxidizing agent that forms in a reaction of nitric oxide (NO•) and superoxide (O2-•). We have

investigated ONOO--induced DNA damage using deoxynucleosides and oligonucleotides as model substrates, with particular attention paid to the oxidation of 8-oxodG by ONOO-. With regard to deoxynucleosides, ONOO- was found to have significant reactivity only with dG, dA, dC, and dT showed minimal reactivity. However, two of the major products of ONOO--induced oxidation of dG (8-oxodG and 8-nitroG) were both found to be significantly more reactive with ONOO- than with dG. In the context of an oligonucleotide, we observed a concentration-dependent oxidation of 8-oxodG to at least

two types of products, one appearing at ONOO- concns. of  $\leq 100 \mu\text{M}$  and the other at concns. of  $\geq 500 \mu\text{M}$ . We also examined the susceptibility of these oxidation products to repair by FaPy glycosylase, endonuclease III, uracil glycosylase, and MutY. FaPy glycosylase, which recognizes 8-oxoG as its primary substrate, was the only enzyme that exhibited an efficient reaction with 8-oxodG oxidation products at low ONOO- concns. ( $\leq 100 \mu\text{M}$ ); the product(s) formed at ONOO- concns. of  $\geq 500 \mu\text{M}$  either was not recognized or was poorly repaired by the enzymes. While processing of the lesions was inefficient with endonuclease III and not apparent with uracil glycosylase, the excision of A opposite an 8-oxoG lesion by the enzyme MutY was not affected by the reaction of 8-oxoG with ONOO-. In addition to demonstrating the complexity of ONOO- DNA damage chemical, these results suggest that 8-oxodG may be a primary target of ONOO- in DNA.

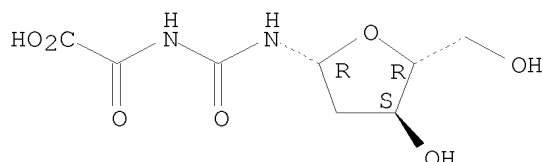
IT 235439-61-9

RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)  
(peroxynitrite-induced oxidation of oxodG)

RN 235439-61-9 CAPLUS

CN Acetic acid, 2-[[[(2-deoxy- $\beta$ -D-erythro-pentofuranosyl)amino]carbonyl]amino]-2-oxo- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 37 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:261266 CAPLUS

DOCUMENT NUMBER: 131:98728

TITLE: Peroxynitrite-induced reactions of synthetic oligonucleotides containing 8-oxoguanine

AUTHOR(S): Tretyakova, Natalia Yu.; Niles, Jacquin C.; Burney, Samar; Wishnok, John S.; Tannenbaum, Steven R.

CORPORATE SOURCE: Division of Bioengineering and Environmental Health and Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Chemical Research in Toxicology (1999), 12(5), 459-466

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

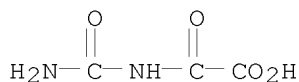
AB 8-Oxoguanine (8-oxo-G) is one of the most common DNA lesions present in normal tissues due to exposure to reactive oxygen species. Studies at this and other labs. suggest that 8-oxo-G is highly susceptible to secondary oxidation, making it a likely target for endogenous oxidizing agents, such as peroxynitrite (ONOO-). Synthetic oligonucleotides containing

8-oxoguanine were treated with ONOO-, and the reaction products were analyzed by liquid chromatog./electrospray ionization mass spectrometry (LC/ESI--MS). CCACAACXCAA, CCAAAGGXAGCAG, CCAAAXGGAGCAG, and TCCCGAGCGGCCAAAGGXAGCAG (X is 8-oxo-G) were found to readily react with peroxyxynitrite via the same transformations as those observed for free 8-oxo-2'-deoxyguanosine. The composition of the reaction mixts. was a function of ONOO- concentration and of the storage time after exposure. The oligonucleotide products isolated at low [ONOO-]/[DNA] ratios (<5) were tentatively assigned as containing 3a-hydroxy-5-imino-3,3a,4,5-tetrahydro-1H-imidazo[4,5d]imidazol-2-one, 5-iminoimidazolidine-2,4-dione, and its hydrolytic product, oxaluric acid. At a [ONOO-]/[DNA] ratio of >10, 2,4,6-trioxo[1,3,5]triazine-1-carboxamide- and cyanuric acid-containing oligomers were the major products. The exact location of a modified base within a DNA sequence was determined using exonuclease digestion of oligonucleotide products followed by LC/ESI--MS anal. of the fragments. For all 8-oxo-G-containing oligomers, independent of the sequence, the reactions with ONOO- took place at the 8-oxo-G residues. These results suggest that 8-oxo-G, if present in DNA, is rapidly oxidized by peroxyxynitrite and that oxaluric acid is a likely secondary oxidation product of 8-oxo-G under physiol. conditions.

IT 585-05-7, Oxaluric acid  
 RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); BIOL (Biological study); FORM (Formation, nonpreparative)  
 (peroxyxynitrite-induced reactions of synthetic oligonucleotides containing 8-oxoguanine)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 38 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:541925 CAPLUS

DOCUMENT NUMBER: 125:267901

ORIGINAL REFERENCE NO.: 125:49849a,49852a

TITLE: Oxidative damage to DNA constituents by iron-mediated Fenton reactions. The deoxycytidine family

AUTHOR(S): Luo, Yongzhang; Henle, Ernst S.; Linn, Stuart

CORPORATE SOURCE: Division Biochemistry Molecular Biology, University California, Berkeley, CA, 94720-3202, USA

SOURCE: Journal of Biological Chemistry (1996), 271(35), 21167-21176  
 CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

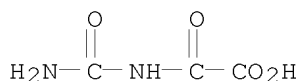
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Damage by iron-mediated Fenton reactions under aerobic or anaerobic conditions to deoxycytidine, deoxycytidine-5'-monophosphate, d-CpC, d-CpCpC, and dCMP residues in DNA resulted in at least 26 distinguishable products. Of these, 24 were identified by high performance liquid chromatog. retention times, radiolabeling, UV absorption spectra, chemical synthesis, fast atom bombardment mass spectrometry, high resolution fast atom bombardment mass spectrometry, and/or NMR. The nature of the products was qual. similar for each substrate except for d-CpC (and possibly d-CpCpC) under anaerobic conditions for which 5-hydroxy-deoxycytidine was uniquely present and 1-carbamoyl-1-carboxy-4-(2-deoxy-β-D-

erythropentofuranosyl)glycinamide was uniquely absent. Damage to dC, d-CpC, and d-CpCpC but not to dCMP or DNA was largely quenched by ethanol, indicating that iron is strongly associated only with dCMP and DNA. The presence of oxygen had little effect with dC or dCMP but had quant. and qual. effects with d-CpC and a significantly quant. but not a qual. effect with DNA. NADH could drive the Fenton reaction to cause damage to the dC family in vitro, consistent with a previous proposal that NADH was the reducing agent for the Fenton reaction in vivo (1988). Finally, the damage spectrum of the dC family by the Fenton reaction is compared with that by ionizing radiation and chemical mechanisms leading to the formation of the 24 identified products are proposed.

IT 585-05-7, Oxaluric acid  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (oxidative damage to DNA constituents by iron-mediated Fenton reactions and deoxycytidine family)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)

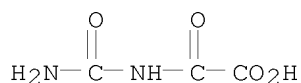


L6 ANSWER 39 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1993:664229 CAPLUS  
 DOCUMENT NUMBER: 119:264229  
 ORIGINAL REFERENCE NO.: 119:47105a,47108a  
 TITLE: Identification of products from oxidation of uric acid induced by hydroxyl radicals  
 AUTHOR(S): Hicks, Mark; Wong, Lisa S.; Day, Richard O.  
 CORPORATE SOURCE: Dep. Clin. Pharmacol. Toxicol., St. Vincent's Hosp., Darlinghurst, 2010, Australia  
 SOURCE: Free Radical Research Communications (1993), 18(6), 337-51  
 CODEN: FRRCEX; ISSN: 8755-0199  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The aim of the present study was to sep. and characterize products formed by oxidation of uric acid by hydroxyl radicals with a view to probing for these products in vivo in clin. contexts. Aerated solns. of 200  $\mu\text{M}$  uric acid, or its oxidation products, allantoin or parabanic acid, were exposed to gamma radiolysis, (52.0 Gy/min), as a source of  $\text{HO}\cdot$  radicals, at pH 3.4 and 7.4. Aliquots were taken every 5 min for 20 min and oxidation products were separated by HPLC and analyzed with a diode array detector. Identities of oxidation products were confirmed on the basis of similarity of retention times and absorbance spectra and peak purity parameters of known stds. Hydroperoxides were measured by tri-iodide formation in the 20-min sample. Exposure of uric acid to such  $\text{HO}\cdot$  fluxes produced a net loss of the parent compound with formation of a complex mixture of products with allantoin and parabanic acid being the predominant products at pH 3.4. The rate of uric acid degradation at physiol. pH was slower and the distribution of oxidation products was different. A small but significant amount of uric acid hydroperoxide was detected at both pHs. A mechanism for uric acid oxidation under these conditions is presented.

IT 585-05-7, Oxaluric acid  
 RL: ANST (Analytical study)  
 (uric acid oxidation product, identification of, by reversed-phase HPLC, pH in relation to)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)





L6 ANSWER 40 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:578807 CAPLUS

DOCUMENT NUMBER: 115:178807

ORIGINAL REFERENCE NO.: 115:30425a,30428a

TITLE: Estimation of standard Gibbs energy changes of biotransformations

AUTHOR(S): Mavrovouniotis, Michael L.

CORPORATE SOURCE: Syst. Res. Cent., Univ. Maryland, College Park, MD, 20742, USA

SOURCE: Journal of Biological Chemistry (1991), 266(22), 14440-5

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Contributions and corrections for the estimation of standard Gibbs energies are

given. The group contribution method, applicable to both cyclic and acyclic compds., permits the approx. estimation of the standard Gibbs energy of a

biotransformation, given the stoichiometry and structures of the metabolites involved. Estimated standard Gibbs energies of formation for a number of

acyclic biochem. compds. are provided.

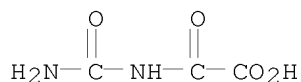
IT 585-05-7

RL: ANST (Analytical study)

(Gibbs energy of formation of, estimation of)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 41 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:488572 CAPLUS

DOCUMENT NUMBER: 115:88572

ORIGINAL REFERENCE NO.: 115:15143a,15146a

TITLE: Spectrophotometric determination of urea-ammonia in the urea degradation pathway of *Saccharomyces cerevisiae*

AUTHOR(S): Low, Christopher; Adams, Bruce G.

CORPORATE SOURCE: Dep. Microbiol., Univ. Hawaii, Manoa, Honolulu, HI, 96822, USA

SOURCE: Journal of Microbiological Methods (1990), 11(3-4), 229-39

CODEN: JMIMDQ; ISSN: 0167-7012

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Titrimetric and spectrophotometric methods demonstrate a modified Berthelot reaction to be a quant. spectrophotometric method specific for  $\text{NH}_3\text{-N}$ . The indophenol chromophore has optimal absorbance at 630 nm (pH 11,  $\text{pK}_a$  8). Spectrophotometric data for urea amidolyase were collected by using a Titertek microplate scanning plate reader, and apparent  $K_m$  values for urea and  $\text{CO}_2$  are in excellent agreement with data obtained with a method employing  $[\text{14C}]\text{urea}$ . The assay is rapid, sensitive, stable, and

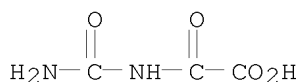
inexpensive, with a lower limit of detection of at least 1  $\mu\text{M}$   $\text{NH}_3$  (14.1 ng  $\text{NH}_3\text{-N/mL}$ ). The assay detects physiol. changes as a function of imposed environment conditions and tests large nos. of samples that yield quant. results with a microplate scanning spectrophotometer.

IT 585-05-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(urea amidolyase of yeast response to)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 42 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:474421 CAPLUS

DOCUMENT NUMBER: 113:74421

ORIGINAL REFERENCE NO.: 113:12505a,12508a

TITLE: 2-Amino-4N-ureidopropionic acid (albizzine) and its oxalyl derivative in hyphae of *Coniophora puteana*

AUTHOR(S): Evans, Christine S.; Burns, Peter J.; Dutton, Martin; Brown, Sarah

CORPORATE SOURCE: Sch. Biol. Sci., Thames Polytech., London, SE18 6PF, UK

SOURCE: Phytochemistry (1990), 29(7), 2159-60

CODEN: PYTCAS; ISSN: 0031-9422

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The non-protein amino acids, albizzine, oxalylalbizzine and 2,3-diaminopropionic acid were isolated from hyphae of *C. puteana*, a wood-rotting basidiomycete causing brown-rot decay.

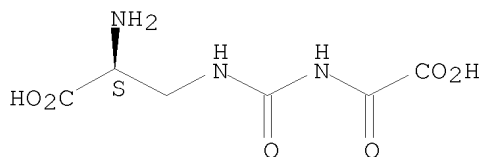
IT 99694-81-2

RL: BIOL (Biological study)  
(from *Coniophora puteana*)

RN 99694-81-2 CAPLUS

CN L-Alanine, 3-[[[(carboxycarbonyl)amino]carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 43 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:210945 CAPLUS

DOCUMENT NUMBER: 112:210945

ORIGINAL REFERENCE NO.: 112:35453a,35456a

TITLE: Action of biologically-relevant oxidizing species upon uric acid. Identification of uric acid oxidation products

AUTHOR(S): Kaur, Harparkash; Halliwell, Barry

CORPORATE SOURCE: King's Coll., Univ. London, London, WC2R 2LS, UK

SOURCE: Chemico-Biological Interactions (1990), 73(2-3), 235-47

CODEN: CBINA8; ISSN: 0009-2797

DOCUMENT TYPE: Journal

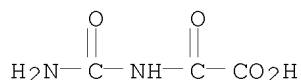
LANGUAGE: English

AB Uric acid is an end-product of purine metabolism in man and an antioxidant  
in vivo. Oxidative products of uric acid were measured by HPLC. Hypochlorous acid rapidly oxidized uric acid, forming allantoin, oxonic/oxaluric and parabanic acids, as well as several unidentified products. HOCl could oxidize all these products further. Hydrogen peroxide did not oxidize uric acid at detectable rates, although it rapidly oxidized oxonic acid and slowly oxidized allantoin and parabanic acids. Hydroxyl radicals generated by hypoxanthine/xanthine oxidase or Fe2+-EDTA/H2O2 systems also oxidized uric acid to allantoin, oxonic/oxaluric acid and traces of parabanic acid. Addition of ascorbic acid to the Fe2+-EDTA/H2O2 system did not increase the formation of oxidation products from uric acid, possibly because ascorbic acid can repair the radicals resulting from the initial attack of hydroxyl radicals upon uric acid. Mixts. of methHb or metmyoglobin and H2O2 also oxidized uric acid: allantoin was the major product, but some parabanic and oxonic/oxaluric acids were also produced. Caeruloplasmin did not oxidize uric acid under physiol. conditions, although simple Cu2+ could, but this was prevented by albumin or histidine. The possibility of using oxidation products of uric acid, such as allantoin, as an index of oxidant generation in vivo in humans is discussed.

IT 585-05-7, Oxaluric acid  
RL: FORM (Formation, nonpreparative)  
(formation of, by oxidation of uric acid)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 44 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:113436 CAPLUS

DOCUMENT NUMBER: 112:113436

ORIGINAL REFERENCE NO.: 112:19099a,19102a

TITLE: The GLN3 gene product is required for transcriptional activation of allantoin system gene expression in *Saccharomyces cerevisiae*

AUTHOR(S): Cooper, Terrance G.; Ferguson, Denise; Rai, Rajendra; Bysani, Nanda

CORPORATE SOURCE: Dep. Microbiol. Immunol., Univ. Tennessee, Memphis, TN, 38163, USA

SOURCE: Journal of Bacteriology (1990), 172(2), 1014-18  
CODEN: JOBAAY; ISSN: 0021-9193

DOCUMENT TYPE: Journal

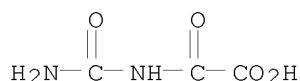
LANGUAGE: English

AB Mutation at the GLN3 locus resulted in decreased steady-state levels of DAL7, DUR1,2, CAR1, and URA3 mRNAs derived from cultures grown in the presence of inducer. Basal levels of these RNA species, however, were not significantly affected by a gln3 mutation. The GLN3 product appears to affect gene expression in 2 ways. The pleiotropic requirement of GLN3 for induced gene expression probably derives from the need of the GLN3 product for inducer uptake into the cell and its loss in gln3 mutants. Transcriptional activation, mediated by the DAL5 and DAL7 upstream activation sequences, requires a functional GLN3 gene product. This observation identified transcriptional activation as the most likely point of GLN3 participation in the expression of allantoin system genes.

IT 585-05-7  
RL: PROC (Process)  
(uptake of, by *Saccharomyces cerevisiae*, gene GLN3 in relation to)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 45 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:95277 CAPLUS

DOCUMENT NUMBER: 112:95277

ORIGINAL REFERENCE NO.: 112:16135a,16138a

TITLE: An inducible allantoinase and the specific toxicity of parabanic acid on allantoin utilization in a Rhizobium species

AUTHOR(S): Rao, N. Venkateswara; Reddy, R. Subhash; Sastry, K. Sivarama

CORPORATE SOURCE: Dep. Biochem., Osmania Univ., Hyderabad, India

SOURCE: Current Microbiology (1990), 20(2), 115-19

CODEN: CUMIDD; ISSN: 0343-8651

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Rhizobium strain NC 92 utilizes uric acid, allantoin, allantoate, urea, and oxaluric acid as sole N sources. Allantoinase is repressible by  $\text{NH}_4^+$  and inducible by allantoin and, less efficiently, by uric acid, oxaluric acid, and allophanate, but not by urea or parabanic acid. This allantoinase (purified .apprx.50-fold to homogeneity) is of 166 Kd mol. weight, is optimally active at pH 7.5, has a  $K_m$  of 4.16 mM and no requirement

for SH groups or metal ions, and is competitively inhibited by acetohydroxamate. Parabanic acid is nontoxic to Rhizobium NC 92 on inorg. N and is highly toxic to growth on allantoin N. Growth inhibition is reversed by supplemented allantoin, and suggestive evidence indicates that NC 92 metabolizes allantoin via the pathway allantoin  $\rightarrow$  allantoate  $\rightarrow$  urea  $\rightarrow$   $\text{NH}_3$ ; allophanate is not an intermediate.

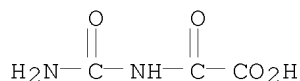
Anal. of allantoinase induction indicates that the mandatory structural requirement is for a free urea moiety in an inducing mol.

IT 585-05-7, Oxaluric acid

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(metabolism of, by Rhizobium)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 46 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:404790 CAPLUS

DOCUMENT NUMBER: 111:4790

ORIGINAL REFERENCE NO.: 111:931a,934a

TITLE: The stepwise mammalian oxidation of the hydantoin 1-methylimidazolidine-2,4-dione into methylimidazolidinetrioxone via 5-hydroxy-1-methylimidazolidine-2,4-dione

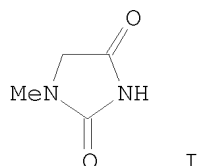
AUTHOR(S): Ienaga, Kazuharu; Nakamura, Ko; Ishii, Akira; Taga, Tooru; Miwa, Yoshihisa; Yoneda, Fumio

CORPORATE SOURCE: Inst. Bio-Active Sci., Nippon Zoki Pharm. Co. Ltd., Hyogo, 673-14, Japan

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (

1989), (6), 1153-6  
CODEN: JCPRB4; ISSN: 0300-922X  
Journal  
English

DOCUMENT TYPE:  
LANGUAGE:  
GI

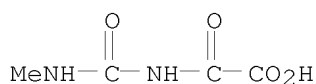


AB The metabolism of 1-methylhydantoin (I) by rabbits is described. The major and general route in mammals proceeds by consecutive oxidns. of I to 5-hydroxy-I and then to 1-methylparabanic acid. Since the 1st oxidation proved to be stereoselective, the step was thought to be enzymic. Although the enantiomeric products could not be separated directly, the mixture was converted into (S)- and (R)-5-(N-Z-L-prolyloxy)-I forms which proved separable and were identified by x-ray anal. of the (R)-diastereoisomer. The ratio of the (S)- to (R)-form was .apprx.3:1. The 2nd product, 1-methylparabanic acid, then undergoes regioselective ring fission to form the methyloxaluric acid (CH<sub>3</sub>NHCONHCOCOOH), which is then hydrolyzed to yield oxalic acid and N-methylurea. Two minor oxidative routes from the substrate I into sarcosine and parabanic acid were also shown to exist.

IT 89281-42-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, methylhydantoin metabolism in relation to)

RN 89281-42-5 CAPLUS

CN Acetic acid, 2-[[ (methyldamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 47 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:131589 CAPLUS

DOCUMENT NUMBER: 110:131589

ORIGINAL REFERENCE NO.: 110:21643a,21646a

TITLE: A simple liquid-chromatographic method for measuring vitamin B6 compounds in plasma

AUTHOR(S): Edwards, Paul; Liu, Peter K. S.; Rose, G. Alan

CORPORATE SOURCE: Biochem. Res. Lab., St. Peter's Hosp., London, WC2, UK

SOURCE: Clinical Chemistry (Washington, DC, United States) (1989), 35(2), 241-5

CODEN: CLCHAU; ISSN: 0009-9147

DOCUMENT TYPE: Journal

LANGUAGE: English

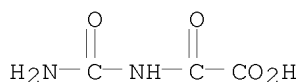
AB A relatively simple reversed-phase HPLC method based on the bisulfite derivatization technique of S. P. Coburn and J. D. Mahuren (1983) was used for measuring all 7 known forms of vitamin B6 in plasma from individuals supplemented with pyridoxine-HCl, and the method showed good anal. recovery (85-98%) and precision. Within-run and between-run relative standard deviations for plasmas supplemented with stds. were 4 and 7%, resp. The major forms of B6 found in unsupplemented plasma from normal subjects were pyridoxal phosphate and 4-pyridoxic acid, with pyridoxal just detectable.

The HPLC procedure correlated well with a modification of an enzymic method involving apotryptophanase for measuring plasma pyridoxal phosphate, and also ( $r = 0.94$ ) with a routine method for determining 4-pyridoxic acid in urine. Elimination of pyridoxine from the plasma of both normal and hyperoxaluric individuals was very rapid, with half-lives of 45 and 40 min, resp. Finally, evidence is presented for the existence of 2 other forms of B6 and the possibility of a new metabolic pathway in vitamin B6 metabolism is discussed.

IT 585-05-7, Oxaluric acid  
 RL: ANST (Analytical study)  
 (metabolic disorders, hyperoxaluria, pyridoxine elimination from blood of human with)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 48 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:92892 CAPLUS

DOCUMENT NUMBER: 110:92892

ORIGINAL REFERENCE NO.: 110:15321a,15324a

TITLE: The metabolism of 1-methylhydantoin via 5-hydroxy-1-methylhydantoin in mammals

AUTHOR(S): Ienaga, Kazuharu; Nakamura, Ko; Naka, Fujio; Goto, Toshio

CORPORATE SOURCE: Inst. Bio-Active Sci., Nippon Zoki Pharm. Co., Ltd., Hyogo, Japan

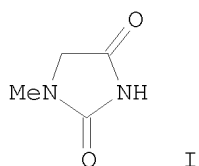
SOURCE: Biochimica et Biophysica Acta, General Subjects (1988), 967(3), 441-3

CODEN: BBGSB3; ISSN: 0304-4165

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

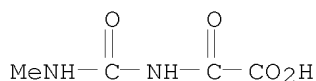


AB The metabolic pathway of 1-methylhydantoin (I) via 5-hydroxy-1-methylhydantoin, methylparabanic acid, and N5-methyloxaluric acid was proven in rabbits and rats. I is not normally formed in healthy animals but may arise from microparasitic creatinine deiminase (EC 3.5.4.21) during infections.

IT 89281-42-5  
 RL: BIOL (Biological study)  
 (as creatinine metabolite formed via methylhydantoin in infection)

RN 89281-42-5 CAPLUS

CN Acetic acid, 2-[[ (methylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 49 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:20383 CAPLUS

DOCUMENT NUMBER: 110:20383

ORIGINAL REFERENCE NO.: 110:3417a,3420a

TITLE: Structural requirements of alloxan and ninhydrin for glucokinase inhibition and of glucose for protection against inhibition

AUTHOR(S): Lenzen, Sigurd; Brand, Franz Hermann; Panten, Uwe

CORPORATE SOURCE: Inst. Pharmacol. Toxicol., Univ. Goettingen, Goettingen, D-3400, Fed. Rep. Ger.

SOURCE: British Journal of Pharmacology (1988), 95(3), 851-9

CODEN: BJPCBM; ISSN: 0007-1188

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Glucose and alloxan competing for the sugar-binding site of glucokinase from pancreatic B-cells or liver was elucidated by determining the structural

requirements of the enzyme for inhibition by alloxan and for protection by glucose. With a half-maximal inhibitory concentration of 5  $\mu\text{M}$ , alloxan was the most potent pyrimidine derivative inhibitor of glucokinase. Uramil was

a less potent enzyme inhibitor. A variety of other pyrimidine derivs. and related substances were ineffective. Ninhydrin also inhibited glucokinase with a half-maximal inhibitory concentration of 5  $\mu\text{M}$ . Isatin was a

slightly less potent enzyme inhibitor. Several other indoline derivs. were ineffective. Only glucose derivs. with a sufficiently bulky substituent in position C-2, such as the glucokinase substrates glucose and mannose and the inhibitors mannoheptulose, glucosamine, and N-acetylglucosamine, protected glucokinase against inhibition by alloxan by binding to the active site of the enzyme. Glucose epimers which differed in other positions did not protect the enzyme against alloxan inhibition. Dithiothreitol protected glucokinase against inhibition by alloxan and reversed the inhibition of the enzyme induced by alloxan. Thus, the mechanism of glucokinase inhibition by alloxan and other inhibitors, such as uramil and ninhydrin, is an oxidation of functionally essential SH groups of the enzyme, where the most reactive keto group of the inhibitor acts as the H acceptor. The protective action of glucose and several C-2 epimers demonstrates that these functionally essential SH groups are situated in the sugar-binding site of the glucokinase. The pancreatic B-cell glucokinase is probably the major target mediating the inhibition of insulin secretion by alloxan.

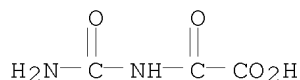
IT 585-05-7, Oxaluric acid

RL: BIOL (Biological study)

(glucokinase of pancreatic  $\beta$ -cell inhibition by, structure in relation to)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 50 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:163813 CAPLUS

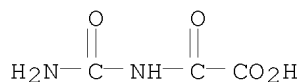
DOCUMENT NUMBER: 108:163813

ORIGINAL REFERENCE NO.: 108:26839a,26842a  
 TITLE: Allantoinases of nodulated *Arachis hypogaea*  
 AUTHOR(S): Rao, N. Venkateswara; Reddy, R. Subhash; Sastry, K. Sivarama  
 CORPORATE SOURCE: Dep. Biochem., Osmania Univ., Hyderabad, India  
 SOURCE: Phytochemistry (1988), 27(3), 693-5  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Nodulated *A. hypogaea* plants contain an allantoinase in the nodules that is different from the host tissue enzyme. The root and nodule allantoinases were purified 10- and 15-fold, resp. They exhibited  $K_m$  values of 25 (root) and 8.7 mM (nodule) for allantoin. Nodule allantoinase exhibits 2 pH optima, a major one at pH 6 and a minor one at pH 4. It is also specifically inhibited by parabanic acid and to a lesser extent by oxaluric acid. *Arachis* Root allantoinase, on the other hand, has 1 pH optimum at pH 7.2 and is not inhibited by parabanic acid or oxaluric acid.

IT 585-05-7, Oxaluric acid  
 RL: BIOL (Biological study)  
 (allantoinase isoform of *Arachis hypogaea* nodule inhibition by, root isoform in relation to)

RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 51 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1987:636345 CAPLUS  
 DOCUMENT NUMBER: 107:236345  
 ORIGINAL REFERENCE NO.: 107:37957a,37960a  
 TITLE: The sonolysis of cytosine and thymine  
 AUTHOR(S): Yu, Tain Jen; Sutherland, Ronald G.; Verrall, Ronald E.  
 CORPORATE SOURCE: Dep. Chem., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.  
 SOURCE: Canadian Journal of Chemistry (1987), 65(6), 1162-4  
 CODEN: CJCHAG; ISSN: 0008-4042  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 107:236345

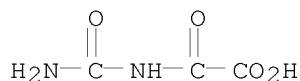
AB Sonolysis of cytosine was studied at 630 kHz in the presence of air and N. The degradation products were identified by gas chromatog.-mass spectral anal.

Under aerated conditions the following products were found: urea, formyl urea, parabanic acid, isobarbituric acid, oxaluric acid, alloxan monohydrate, alloxantin, dialuric acid, and uracil glycols. Under N the degradation products were isobarbituric acid, alloxan monohydrate, and uracil glycols. Sonolysis of thymine in the presence of air was reinvestigated and a previously reported, unidentified, product may be 5-hydroxy-5-methylbarbituric acid. A mechanism for the sonolytic degradation of cytosine is proposed.

IT 585-05-7P, Oxaluric acid  
 RL: FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation of, in sonolysis of cytosine)

RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)





L6 ANSWER 52 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:632807 CAPLUS

DOCUMENT NUMBER: 107:232807

ORIGINAL REFERENCE NO.: 107:37343a,37346a

TITLE: Allantoin transport in *Saccharomyces cerevisiae* is regulated by two induction systems

AUTHOR(S): Cooper, Terrance G.; Chisholm, Vanessa T.; Cho, Hyo Jeong; Yoo, Hyang Sook

CORPORATE SOURCE: Dep. Microbiol. Immunol., Univ. Tennessee, Memphis, TN, 38163, USA

SOURCE: Journal of Bacteriology (1987), 169(10), 4660-7

CODEN: JOBAA; ISSN: 0021-9193

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The allantoin transport system of *S. cerevisiae* responds to two induction systems, one mediated by allophanate or its analog oxalurate and the other mediated by allantoin or its analog hydantoin acetate. The effects of the two inducers were additive in strain M85. Like other allantoin pathway genes, oxalurate-mediated induction of allantoin transport required a functional Dal81 gene product. Hydantoin acetate-mediated induction of the system, on the other hand, occurred normally in dal81 mutants. This suggests that induction was not only mediated by two sep. inducers, but also involved different regulatory proteins. Induction is probably a transcriptionally regulated process, because addition of hydantoin acetate

or

oxalurate to the culture medium increased the steady-state levels of mRNA encoded by a gene required for allantoin transport (Dal4).

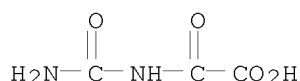
IT 585-05-7

RL: BIOL (Biological study)

(allantoin transport system induction by, *Saccharomyces cerevisiae* gene DAL81 in)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 53 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:587351 CAPLUS

DOCUMENT NUMBER: 105:187351

ORIGINAL REFERENCE NO.: 105:30173a,30176a

TITLE: Control of enzyme synthesis in the oxalurate catabolic pathway of *Streptococcus faecalis* ATCC 11700: evidence for the existence of a third carbamate kinase

AUTHOR(S): Vander Wauven, Corinne; Simon, Jean Paul; Slos, Philippe; Stalon, Victor

CORPORATE SOURCE: Inst. Rech., CERIA, Belg.

SOURCE: Archives of Microbiology (1986), 145(4), 386-90

CODEN: AMICCW; ISSN: 0302-8933

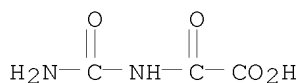
DOCUMENT TYPE: Journal

LANGUAGE: English

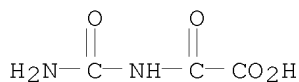
AB *S. faecalis* ATCC 11700 uses oxalurate as a sole energy source for growth. An oxamate carbamoyltransferase and a carbamate kinase, both induced by

oxalurate, are involved in this process. The oxalurate-induced kinase is specific for the pathway. Its properties are different from those of the previously characterized agmatine- and arginine-induced kinases. Glucose, but not arginine nor agmatine, 2 other energy sources, represses the oxalurate pathway. In contrast, oxalurate was at least as effective as glucose in repressing the arginine deiminase pathway in arginine-grown cells, or the agmatine deiminase pathway during growth on agmatine.

IT 585-05-7  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (metabolism of, by *Streptococcus faecalis*, carbamate kinase activity in)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



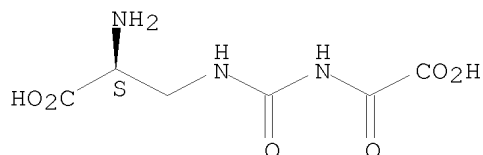
L6 ANSWER 54 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1986:421424 CAPLUS  
 DOCUMENT NUMBER: 105:21424  
 ORIGINAL REFERENCE NO.: 105:3545a,3548a  
 TITLE: Dual regulation of the allantoin permease in *Saccharomyces cerevisiae*  
 AUTHOR(S): Cooper, Terrance G.; Chisholm, Vanessa T.; Cho, Hyo Jeong; Yoo, Hyang Sook  
 CORPORATE SOURCE: Cent. Health Sci., Univ. Tennessee, Memphis, TN, 38163, USA  
 SOURCE: Microbiology (Washington, D. C.) (1986) 242-5  
 CODEN: MICRDG; ISSN: 0098-1540  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Allantoin transport in *S. cerevisiae* was induced by oxalurate and hydantoin acetate. The ability of oxalurate to support induction required DAL81 gene product that was required for induction of the allantoin pathway enzymes. In contrast, induction by hydantoin acetate did not require participation of Dal81 gene. This suggested that the allantoin transport system is regulated by a dual induction system consisting of 2 inducers which operate via 2 sep. regulatory systems consisting of different elements. Cloning and expression of DAL4 gene are reviewed and discussed.  
 IT 585-05-7  
 RL: BIOL (Biological study)  
 (allantoin transport by *Saccharomyces cerevisiae* induction by)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



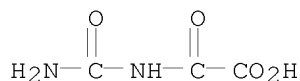
L6 ANSWER 55 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1986:31737 CAPLUS  
 DOCUMENT NUMBER: 104:31737  
 ORIGINAL REFERENCE NO.: 104:5157a,5160a  
 TITLE: 2-Amino-4-acetylaminobutyric acid, 2,4-diaminobutyric acid and 2-amino-6N-oxalylureidopropionic acid (oxalylalbizziine) in seeds of *Acacia angustissima*  
 AUTHOR(S): Evans, Christine S.; Clardy, Jon; Hughes, Philip F.;

Bell, E. Arthur  
 CORPORATE SOURCE: Sch. Biol. Sci., Thames Polytech., London, SE18 6PF, UK  
 SOURCE: Phytochemistry (Elsevier) (1985), 24(10), 2273-5  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A new amino acid previously detected in 17 species of Acacia was isolated from seeds of *A. angustissima* and identified as oxalylalbizziine. These seeds also contain >6% dry weight of 2-amino-4-acetylaminobutyric acid, which has not been reported previously in a legume, and lower concns. of 2,4-diaminobutyric acid.  
 IT 99694-81-2  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)  
 (of *Acacia angustissima*, isolation and structure of)  
 RN 99694-81-2 CAPLUS  
 CN L-Alanine, 3-[[[(carboxycarbonyl)amino]carbonyl]amino]- (CA INDEX NAME)

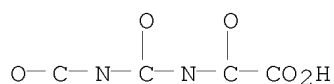
Absolute stereochemistry.



L6 ANSWER 56 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1983:212395 CAPLUS  
 DOCUMENT NUMBER: 98:212395  
 ORIGINAL REFERENCE NO.: 98:32243a,32246a  
 TITLE: Reduction of oxalogenesis in a rapid gas chromatographic procedure for the analysis of oxalate ion in urine  
 AUTHOR(S): Moye, H. Anson; Malagodi, Marjorie H.; Clarke, Dorothy H.  
 CORPORATE SOURCE: Dep. Food Sci. Hum. Nutr., Univ. Florida, Gainesville, FL, 32611, USA  
 SOURCE: Clinica Chimica Acta (1983), 129(3), 385-90  
 CODEN: CCATAR; ISSN: 0009-8981  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Enzymic degradation of urinary oxalic acid by oxalate decarboxylase prior to derivatization was used to document the contribution of oxalogenic compds., e.g., oxamic acid, oxaluric acid, and parabanic acid, to the oxalic acid measured by the gas chromatog. method of H. A. Moye et al. (1981), and a modified method was developed which minimized interference from the oxalogenic compds. When derivatization was done at 25° or 80°, all compds. examined produced GC peaks having the same retention as the bis-2-chloroethyl ester of oxalic acid. However, conversion was significantly greater at 80° (30 min), and this was probably due to heat-induced conversion of the oxalogenic compds. to oxalic acid. Therefore, the original derivatization conditions (80° for 30 min) were changed to 25° for 60 min.  
 IT 585-05-7  
 RL: ANST (Analytical study)  
 (interference by, in oxalate determination in human urine by gas chromatog.)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



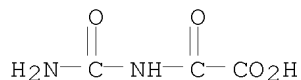
L6 ANSWER 57 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1982:77430 CAPLUS  
 DOCUMENT NUMBER: 96:77430  
 ORIGINAL REFERENCE NO.: 96:12603a,12606a  
 TITLE: On the ESR detection of the  $\sigma$ -radical  
 RNHCO $\cdot$  in irradiated crystals of  
 5,5-dihydroxybarbituric acid (alloxan) trihydrate  
 AUTHOR(S): Sagstuen, Einar; Skjaervoe, Halvard  
 CORPORATE SOURCE: Inst. Phys., Univ. Oslo, Oslo, Norway  
 SOURCE: Journal of Chemical Physics (1981), 75(12),  
 5627-9  
 CODEN: JCPSA6; ISSN: 0021-9606  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB In single crystals of 5,5-dihydroxybarbituric acid (alloxan) trihydrate,  
 an ESR absorption was observed after irradiation at 77 K which is ascribed  
 to the  $\sigma$ -radical RNHCO. Its spectral parameters are described and compared  
 to those from the structurally similar  $\sigma$ -acyl radical in malonic and  
 succinic acid. The radical is formed from the primary oxidation product  
 RCO.(OH) through electronic rearrangements leading to an opening of the  
 pyrimidine ring.  
 IT 80731-17-5P  
 RL: PREP (Preparation)  
 (formation and ESR detection of, in irradiated single crystals of  
 alloxan trihydrate)  
 RN 80731-17-5 CAPLUS  
 CN Methyl, [[[(carboxycarbonyl)amino]carbonyl]amino]oxo- (9CI) (CA INDEX  
 NAME)



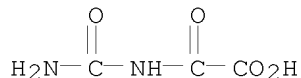
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L6 ANSWER 58 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1982:3411 CAPLUS  
 DOCUMENT NUMBER: 96:3411  
 ORIGINAL REFERENCE NO.: 96:611a,614a  
 TITLE: L-Ornithine transaminase synthesis in *Saccharomyces*  
*cerevisiae*: induction by allophanate, intermediate  
 and inducer of the urea degradative pathway adds to  
 arginine induction  
 AUTHOR(S): Hennaut, Claudette  
 CORPORATE SOURCE: Inst. Rech., CERIA, Brussels, B-1070, Belg.  
 SOURCE: Current Genetics (1981), 4(1), 69-72  
 CODEN: CUGED5; ISSN: 0172-8083  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Yeast ornithine transaminase is induced by arginine and ornithine, through  
 the action of regulatory elements common to arginase induction. Ornithine  
 transaminase is subject to a 2nd induction circuit, that which is  
 responsible for urea amidolyase and urea permease induction by allophanate  
 and defined by the regulatory mutants *durL*- and *durM*-.  
 IT 585-05-7  
 RL: BIOL (Biological study)

(ornithine transaminase induction by, in *Saccharomyces cerevisiae*)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 59 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1981:421015 CAPLUS  
DOCUMENT NUMBER: 95:21015  
ORIGINAL REFERENCE NO.: 95:3653a,3656a  
TITLE: Repression of catabolic NAD-specific glutamate dehydrogenase of *Saccharomyces cerevisiae* by arginine, allantoin and urea  
AUTHOR(S): Middelhoven, W. J.; Hoogkamer-Te Niet, Mieke C.  
CORPORATE SOURCE: Lab. Microbiol., Landbouwhogeschool, Wageningen, 6703 CT, Neth.  
SOURCE: FEMS Microbiology Letters (1981), 10(4), 307-11  
CODEN: FMLED7; ISSN: 0378-1097  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The repression of NAD-specific glutamate dehydrogenase (GDH-B) by allantoin, arginine, and urea was examined in *S. cerevisiae* wild-type and mutant strains during growth on L-alanine, 4-aminobutyric acid, L-aspartic acid, L-glutamic acid, and L-proline as sole N sources. Allantoin, arginine, and urea were low-mol.-weight repressors of GDH-B; no further metabolism to NH<sub>3</sub> and glutamine was required for repression. GDH-B formation was also repressed by the nonmetabolizable analogs homoarginine, hydantoate, and oxalurate. Repression of GDH-B by arginine was independent of gene *argR*. Patterns of repression suggested that simultaneous intracellular accumulation of arginine and urea was required for significant repression of GDH-B in the presence of 4-aminobutyric acid. The biochem. of GDH-B repression is discussed.  
IT 585-05-7  
RL: BIOL (Biological study)  
(NAD-specific glutamate dehydrogenase repression by, in *Saccharomyces cerevisiae*)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 60 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1981:98145 CAPLUS  
DOCUMENT NUMBER: 94:98145  
ORIGINAL REFERENCE NO.: 94:15939a,15942a  
TITLE: The sonolysis of uracil  
AUTHOR(S): Yu, Tain-Jen; Sutherland, Ronald G.; Verrall, Ronald E.  
CORPORATE SOURCE: Dep. Chem. Chem. Eng., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.  
SOURCE: Canadian Journal of Chemistry (1980), 58(18), 1909-15  
CODEN: CJCHAG; ISSN: 0008-4042  
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The sonolysis of uracil was studied at 630 kHz in the presence of air, O, N, and Ar. The degradation products were identified by gas chromatog.-mass spectrometry anal. Under aerated conditions the following products were found: uracil glycols (I), isobarbituric acid (II), N-formyl-N'-glyoxyurea (III), 5-hydroxyhydantoin (IV), dialuric acid (V), alloxan monohydrate (VI), parabanic acid (VII), and oxaluric acid (VIII). In deaerated solns., III, VII, and VIII were not observed, but either 6-hydroxy-5,6-dihydrouracil or its isomer were detected in addition to I, II, IV, V, and VI. The observed products were used to develop a possible mechanism for the sonolytic degradation and the results are similar to those obtained in radiolysis. The sonolytic degradation of 5-bromouracil is also reported;

the products observed were 5-bromobarbituric acid, IV, VI, VII, and VIII, and these can be rationalized by a similar mechanistic scheme.

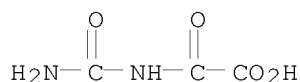
IT 585-05-7

RL: BIOL (Biological study)

(as uracil sonolytic degradation product)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 61 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:634263 CAPLUS

DOCUMENT NUMBER: 93:234263

ORIGINAL REFERENCE NO.: 93:37443a,37446a

TITLE: Analytical isotachophoresis: a rapid and sensitive method for determination of urinary oxalate

AUTHOR(S): Schmidt, K.; Hagmaier, V.; Bruchelt, G.; Rutishauser, G.

CORPORATE SOURCE: Dep. Surg., Univ. Tuebingen, Tuebingen, D-7400, Fed. Rep. Ger.

SOURCE: Urological Research (1980), 8(3), 177-80

CODEN: URLRA5; ISSN: 0300-5623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complete separation of the oxalate anion from accompanying ions is achieved in

an 800 + 0.5 mm PTFE capillary between 2 electrodes according to differences in the net mobility. To lower the ionic strength of urine and reduce anal. time, oxalate was precipitated by CaCl<sub>2</sub> before anal. The

separated compds. were detected by thermosignal and UV absorbance at 254 nm. Short anal. time, little pretreatment of the urine samples, and high resolving power and accuracy are the significant advantages of this newly developed method. This new technique was of significant value in studying the role of oxalate in urinary stone disease.

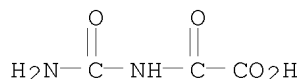
IT 585-05-7

RL: ANT (Analyte); ANST (Analytical study)

(detection of, in urine by isotachophoresis)

RN 585-05-7 CAPLUS

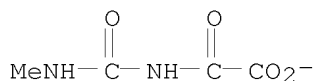
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 62 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1980:408132 CAPLUS  
 DOCUMENT NUMBER: 93:8132  
 ORIGINAL REFERENCE NO.: 93:1495a,1498a  
 TITLE: Activation and transfer of oxygen. XV. Evidence for  
 the transient opening of the pyrazine ring in N1- and  
 N5-alkylflavin models, 4A- to 10A-Adduct  
 isomerization and pyrazine and pyrimidine ring  
 contractions  
 AUTHOR(S): Mager, H. I. X.  
 CORPORATE SOURCE: Biochem. Biophys. Lab., Univ. Technol., Delft, 2628  
 BC, Neth.  
 SOURCE: Tetrahedron Letters (1979), (37), 3549-52  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

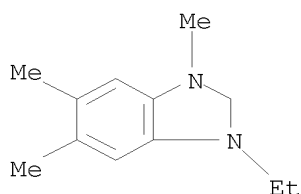
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The equilibrium of the hydroxy pseudobase I with the blue intermediate II  
 was confirmed by the isolation of 1-methylbenzimidazole from spontaneously  
 bleached solns. of II. Similarly, the flavinium cation III with OH- gave  
 the 4a-adduct IV which underwent ring contraction to the spirohydantoin V  
 via a carbonyl oxide, isomerization to the 10a-adduct VI, and pyrazine  
 ring cleavage and contraction to the benzimidazolinium salts VII and VIII.  
 VII and VIII are also formed from VI. VI also underwent ring contraction  
 to the spirohydantoin IX.  
 IT 73813-80-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 73813-80-6 CAPLUS  
 CN 1H-Benzimidazolium, 1-ethyl-3,5,6-trimethyl-, salt with  
 [[(methylamino)carbonyl]amino]oxoacetic acid (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 73813-79-3  
 CMF C4 H5 N2 O4



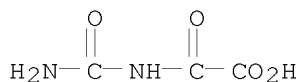
CM 2

CRN 73813-78-2  
 CMF C12 H17 N2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L6 ANSWER 63 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1979:589498 CAPLUS  
DOCUMENT NUMBER: 91:189498  
ORIGINAL REFERENCE NO.: 91:30475a,30478a  
TITLE: Oxalurate transport in *Saccharomyces cerevisiae*  
AUTHOR(S): Cooper, Terrance G.; McKelvey, Joyce; Sumrada, Roberta  
CORPORATE SOURCE: Dep. Biol. Sci., Univ. Pittsburgh, Pittsburgh, PA,  
15260, USA  
SOURCE: Journal of Bacteriology (1979), 139(3),  
917-23  
CODEN: JOBAA; ISSN: 0021-9193  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Oxalurate, the gratuitous inducer of the allantoin degradative enzymes,  
was taken into the yeast cell by an energy-dependent active transport  
system with an apparent  $K_m$  of 1.2 mM. Efflux of previously accumulated  
oxalurate was rapid, with a half-life of approx. 2 min. The oxalurate  
uptake system appears to be both constitutively produced and insensitive  
to N catabolite repression. The latter observations suggest that failure  
of oxalurate to bring about induction of allophanate hydrolase in cultures  
growing under repressive conditions does not result from inducer  
exclusion, but rather from repression of *durl2* gene expression.  
IT 585-05-7  
RL: PROC (Process)  
(transport of, in *Saccharomyces cerevisiae*)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



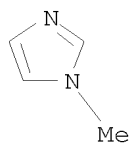
L6 ANSWER 64 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1979:144533 CAPLUS  
DOCUMENT NUMBER: 90:144533  
ORIGINAL REFERENCE NO.: 90:22840h,22841a  
TITLE: [Crystal structure of] 1-methylimidazolium oxalurate  
AUTHOR(S): Wang, Albert C.; Craven, B. M.  
CORPORATE SOURCE: Crystallogr. Dep., Univ. Pittsburgh, Pittsburgh, PA,  
USA  
SOURCE: Acta Crystallographica, Section B: Structural  
Crystallography and Crystal Chemistry (1979  
) , B35(2), 510-13  
CODEN: ACBCAR; ISSN: 0567-7408  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The title compound is triclinic, space group  $P_{21}2121$ , with  $a$  7.718(4),  $b$   
8.062(4),  $c$  9.603(4) Å,  $\alpha$  69.34(4),  $\beta$  62.52(4), and  $\gamma$   
67.22(4)°;  $d(\text{exptl.}) = 1.490$  for  $Z = 2$ . The structure determination was  
based on the x-ray intensities (Mo  $K\alpha$ ) of 1779 reflections collected  
by diffractometer. Parameter refinement by the full-matrix least-squares  
method gave  $R = 0.058$ . The longer carboxylate C-O bond (1.259 vs. 1.230  
Å) involves the O atom which forms the salt bridge (NH...O 2.78 Å)  
and another H bond.  
IT 69723-06-4  
RL: PRP (Properties)  
(crystal structure of)  
RN 69723-06-4 CAPLUS  
CN Acetic acid, [(aminocarbonyl)amino]oxo-, compd. with 1-methyl-1H-imidazole  
(1:1) (9CI) (CA INDEX NAME)



CM 1

CRN 616-47-7

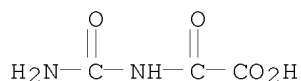
CMF C4 H6 N2



CM 2

CRN 585-05-7

CMF C3 H4 N2 O4



L6 ANSWER 65 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:85431 CAPLUS

DOCUMENT NUMBER: 88:85431

ORIGINAL REFERENCE NO.: 88:13401a,13404a

TITLE: Separation of low-molecular weight purine electrooxidation products from phosphate buffers

AUTHOR(S): Owens, James L.; Thomas, Hazel H.; Dryhurst, Glenn

CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, USA

SOURCE: Analytica Chimica Acta (1978), 96(1), 89-97

CODEN: ACACAM; ISSN: 0003-2670

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two chromatog. methods were developed to sep. quant. a number of organic compds.

such as alloxan, urea, allantoin, parabanic acid, oxaluric acid, and D-ribose from relatively large amts. of inorg. phosphate. These organic compds. are representative of typical products expected upon electrochem. oxidation of various purine derivs. that may be themselves separated from

each

other by liquid chromatog. with phosphate buffers. The phosphate may subsequently be separated from the organic components either by use of a

Sephadex

G 10 gel permeation column with water or very dilute HCl as the eluant or by use of a MeOH-washed column of a strong cation-exchange resin with MeOH as eluant.

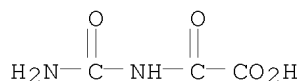
IT 585-05-7

RL: ANST (Analytical study)

(separation of, from inorg. phosphate, chromatog.)

RN 585-05-7 CAPLUS

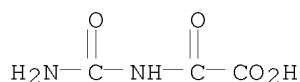
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



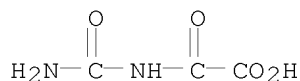
L6 ANSWER 66 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:34018 CAPLUS

DOCUMENT NUMBER: 88:34018  
 ORIGINAL REFERENCE NO.: 88:5351a,5354a  
 TITLE: Liquid chromatographic separation of electrochemical oxidation products of biologically important purines  
 AUTHOR(S): Cleary, Michael T.; Dryhurst, Glenn  
 CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, USA  
 SOURCE: Analytica Chimica Acta (1977), 94(2), 343-50  
 CODEN: ACACAM; ISSN: 0003-2670  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A liquid chromatog. method that uses a dual column system (Sephadex G 10 gel permeation and Sephadex QAE A 25 anion exchange) was developed for the quant. separation of mixts. of compds. found as products of electrochem. oxidation of biol. important purines. Small quantities (mg range) of such product mixts. may be separated, and quant. anal. also is possible in some case.  
 IT 585-05-7  
 RL: ANST (Analytical study)  
 (separation and determination of, dual-column chromatog. for, purine oxidation in relation to)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



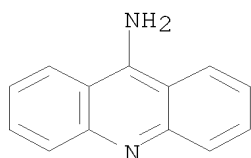
L6 ANSWER 67 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1976:405473 CAPLUS  
 DOCUMENT NUMBER: 85:5473  
 ORIGINAL REFERENCE NO.: 85:875a,878a  
 TITLE: Preparation of aminoacridine salts  
 AUTHOR(S): Petyunin, G. P.; Sysun, V. N.  
 CORPORATE SOURCE: Khar'k. Farm. Inst., Kharkov, USSR  
 SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1975), 9(7), 24-8  
 CODEN: KHFFZAN; ISSN: 0023-1134  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI For diagram(s), see printed CA Issue.  
 AB 9-Aminoacridine (I) salts, e.g., I.RO2CCO2H (R = Et, Pr, Bu, octyl, PhCH2), II.RO2CCO2H (Me, CH2CH2Cl, Pr, Me2CH, Bu, pentyl, hexyl, heptyl, nonyl), I.RNHCOCO2H (R = Ph, p-MeC6H4, p-ClC6H4, o-, p-MeOC6H4, p-O2NC6H4, o-MeO2CC6H4, p-EtO2CC6H4, NH2CO, 2-, 3-, 4-pyridyl, 3-, 8-quinolyl), I.RNHNHCOCO2H (R = Ph, o-, m-, p-MeC6H4, o-, m-BrC6H4, m-, p-ClC6H4, o-MeOC6H4), and I.RCH:NNHCOCO2H [R = Ph, p-O2NC6H4, 3,4-(MeO)2C6H3] were obtained in 55-96% yields by mixing equimol. quantities of the acridine with the corresponding acid 24 hr at room temperature or by heating 30-40 min on a water bath.  
 IT 57727-31-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 57727-31-8 CAPLUS  
 CN Acetic acid, [(aminocarbonyl)amino]oxo-, compd. with 9-acridinamine (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 585-05-7  
 CMF C3 H4 N2 O4



CM 2

CRN 90-45-9

CMF C13 H10 N2



L6 ANSWER 68 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:571163 CAPLUS

DOCUMENT NUMBER: 83:171163

ORIGINAL REFERENCE NO.: 83:26795a,26798a

TITLE: X-ray crystal structure of the molecular complex  
9-ethyladenine-parabanic acid-oxaluric acid  
monohydrate

AUTHOR(S): Shieh, Huey-Sheng; Voet, Donald

CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, USA

SOURCE: Acta Crystallographica, Section B: Structural  
Crystallography and Crystal Chemistry (1975  
, B31(9), 2192-201

CODEN: ACBCAR; ISSN: 0567-7408

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Crystals of the complex 9-ethyladenine-parabanic acid-oxaluric acid monohydrate, C13H17N9O8, have space group P.hivin.1, with a 6.802(1), b 13.131(2), c 11.135(2) Å, α 98.03(1), β 112.53(1), γ 98.04(1)°, and Z = 2. Intensity data were measured with an automated diffractometer using graphite monochromated Cu Kα radiation. The structure was solved by direct methods and refined by full matrix least-squares procedures to a final R = 0.040 based on 2808 unique reflections. The structure consists of roughly planar layers of mols. that are extensively H bonded to one another. The parabanic acid carbonyl groups exhibit little, if any, tendency to act as H-bond acceptors. Adjacent layers of mols. stack so that there are several interatomic contacts less than the minimal van der Waals distance. These close approaches appear to be due to Coulomb interactions involving ionic charges and strong dipoles. The role of the water mol. seems to be largely that of filling a cavity in the crystal structure.

IT 57228-63-4

RL: PRP (Properties)  
(crystal structure of)

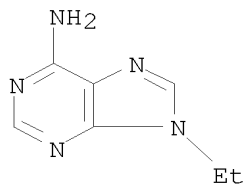
RN 57228-63-4 CAPLUS

CN Acetic acid, [(aminocarbonyl)amino]oxo-, compd. with 9-ethyl-9H-purin-6-amine and imidazolidinetriene (1:1:1), monohydrate (9CI) (CA INDEX NAME)

CM 1

CRN 2715-68-6

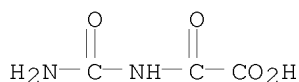
CMF C7 H9 N5



CM 2

CRN 585-05-7

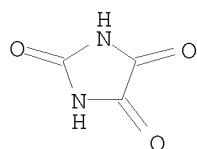
CMF C3 H4 N2 O4



CM 3

CRN 120-89-8

CMF C3 H2 N2 O3



L6 ANSWER 69 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:401164 CAPLUS

DOCUMENT NUMBER: 81:1164

ORIGINAL REFERENCE NO.: 81:195a,198a

TITLE: Oxaluric acid. Nonmetabolizable inducer of the allantoin degradative enzymes in *Saccharomyces cerevisiae*

AUTHOR(S): Sumrada, Roberta; Cooper, Terrance G.

CORPORATE SOURCE: Fac. Arts Sci., Univ. Pittsburgh, Pittsburgh, PA, USA

SOURCE: Journal of Bacteriology (1974), 117(3), 1240-7

CODEN: JOBAAY; ISSN: 0021-9193

DOCUMENT TYPE: Journal

LANGUAGE: English

AB *S. cerevisiae* degrades allantoin in 5 steps to NH<sub>3</sub>, CO<sub>2</sub>, and glyoxylate. It is known that allophanic acid, the last intermediate of the pathway, is required for induction of all 5 degradation enzymes. The data indicate that oxaluric acid, an allophanate analog, can serve as a nonmetabolizable inducer. Oxaluric acid causes a high level of induction even in strains lacking urea carboxylase.

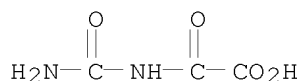
IT 585-05-7

RL: BIOL (Biological study)

(allantoin degradation enzymes induction by, in *Saccharomyces cerevisiae*)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 70 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:133745 CAPLUS

DOCUMENT NUMBER: 80:133745

ORIGINAL REFERENCE NO.: 80:21577a,21580a

TITLE: Gamma irradiation of cytosine in an aerated aqueous solution. I. Identification of radiolysis products of cytosine resulting from the deamination pathway

AUTHOR(S): Polverelli, M.; Teoule, R.

CORPORATE SOURCE: Dep. Rech. Fondam., C.E.N., Grenoble, Fr.

SOURCE: Zeitschrift fuer Naturforschung, Teil C: Biochemie, Biophysik, Biologie, Virologie (1974), 29(1-2), 12-15

CODEN: ZNFCAP; ISSN: 0341-0471

DOCUMENT TYPE: Journal

LANGUAGE: English

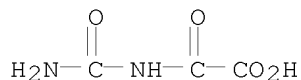
AB Radiolysis products resulting from the deamination pathway were isolated and identified after irradiation of cytosine with  $\gamma$ -rays in neutral aqueous solns. They were identical to those identified in uracil radiolysis, i.e. 5-6-dihydroxy-5,6-dihydrouracil (cis and trans forms), isodialuric acid, alloxan, 5-hydroxyhydantoin, parabanic acid, and oxaluric acid. The absence of 4,4'-diisobarbituric acid, alloxantin, or isobarbituric acid could be explained by the good stability of uracil glycols. The identification of biuret proved potential degradation mechanisms different from those involving the free radical attack on the 5,6-double bond.

IT 585-05-7P

RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, from radiolytic degradation of cytosine)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 71 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:131928 CAPLUS

DOCUMENT NUMBER: 78:131928

ORIGINAL REFERENCE NO.: 78:21143a,21146a

TITLE: GABA [ $\gamma$ -aminobutyric acid] uptake in rat brain slices. Inhibition by GABA analogs and by various drugs

AUTHOR(S): Beart, P. M.; Johnston, G. A. R.

CORPORATE SOURCE: Dep. Physiol., Aust. Natl. Univ., Canberra, Australia

SOURCE: Journal of Neurochemistry (1973), 20(2), 319-24

CODEN: JONRA9; ISSN: 0022-3042

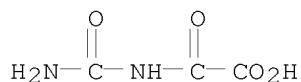
DOCUMENT TYPE: Journal

LANGUAGE: English

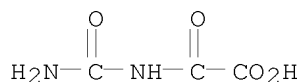
AB Of 77 compds. tested, 2-hydroxy-4-aminobutyric acid [3938-83-8] was the most potent inhibitor of  $\gamma$ -aminobutyric acid [56-12-2] uptake by rat brain slices in vitro. It and the other GABA analogs tested (2-chloro-4-aminobutyric acid [39919-02-3], 2-methyl-4-aminobutyric acid [39919-03-4], and 4-methyl-4-aminobutyric acid [627-61-2]) were competitive inhibitors of GABA uptake by the slices. A number of drugs such as amiloride [2609-46-3] and bicuculline methochloride [38641-83-7] nonspecifically inhibited GABA uptake.

IT 585-05-7

RL: BIOL (Biological study)  
 (GABA uptake by brain inhibition by)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)

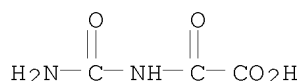


L6 ANSWER 72 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1973:39964 CAPLUS  
 DOCUMENT NUMBER: 78:39964  
 ORIGINAL REFERENCE NO.: 78:6297a,6300a  
 TITLE: Radiation effects induced by  $\gamma$ -radiation of pyrimidines in aqueous solutions  
 AUTHOR(S): Pleticha-Lansky, R.  
 CORPORATE SOURCE: Inst. Exp. Bot., Prague, Czech.  
 SOURCE: Tsitologiya i Genetika (1972), 6(5), 400-9  
 CODEN: TGANAK; ISSN: 0564-3783  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB Investigations with polarog., oscillopolarog., chromatog., and  $^{14}\text{C}$ -labeled pyrimidines showed that, as a result of  $\gamma$ -irradiation of cytosine and uracil in aqueous solns. isobarbituric, 4,4'-diisobarbituric, and isodialuric acids and the system, dialuric acid + alloxan .dblarw. alloxantin were formed. As a result of their hydrolysis, parabanic and oxaluric acids are formed. Mechanisms of the chemical and radiation-chemical processes are discussed.  
 IT 585-05-7  
 RL: FORM (Formation, nonpreparative)  
 (formation of, from radiolysis of pyrimidines)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 73 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1971:434132 CAPLUS  
 DOCUMENT NUMBER: 75:34132  
 ORIGINAL REFERENCE NO.: 75:5393a,5396a  
 TITLE: Radical reaction of food constituents. Photolysis of uracil in the presence of hydrogen peroxide  
 AUTHOR(S): Ochiai, Hideo  
 CORPORATE SOURCE: Coll. Agric., Shimane Univ., Shimane, Japan  
 SOURCE: Agricultural and Biological Chemistry (1971), 35(4), 622-4  
 CODEN: ABCHA6; ISSN: 0002-1369  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Upon irradiation with uv-light in the presence of  $\text{H}_2\text{O}_2$ , uracil was decomposed to parabanic acid and oxaluric acid. Oxaluric acid was further decomposed to urea and oxalic acid.  
 IT 585-05-7  
 RL: FORM (Formation, nonpreparative)  
 (formation of, in uracil decomposition by uv light)  
 RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 74 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:74901 CAPLUS

DOCUMENT NUMBER: 68:74901

ORIGINAL REFERENCE NO.: 68:14411a,14414a

TITLE: Polarographic reduction of oxaluric acid. Analytical application

AUTHOR(S): Dryhurst, Glenn; Elving, Philip J.

CORPORATE SOURCE: Univ. of Michigan, Ann Arbor, MI, USA

SOURCE: Analytical Chemistry (1968), 40(3), 492-5

CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The polarographic reduction of oxaluric acid (I) in a 2-electron process, apparently to glyoxylic acid monoureide, is studied. At pH 1-5, undissocd. I is reduced, giving a single, well-formed polarographic wave. At pH 1-6, the half-wave potential,  $E_{1/2}$ , varies linearly with pH according to the equation  $E_{1/2} = -0.895 - 0.108 \text{ pH}$ . At pH >6.1, a single, essentially pH-independent wave is obtained at  $E_{1/2} = -1.650 \pm 0.080$ , corresponding to the reduction of the oxalurate anion. At pH 5-6, both processes occur, the heights of the resp. waves depending on the extent of I dissociation and the rate of recombination of the anion and  $\text{H}^+$ . The anal. application of the polarographic reduction of I is discussed. In pH 0.75

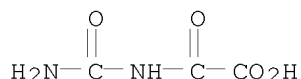
Cl- and pH 4.7 OAc- media, a nearly linear dependence of concentration on wave height is obtained for 0.2-1.0mM I. The deviation of the limiting current values at each concentration is  $\pm 3\%$  of the mean.

IT 585-05-7

RL: ANT (Analyte); ANST (Analytical study)  
(determination of, polarographic)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 75 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:344 CAPLUS

DOCUMENT NUMBER: 66:344

ORIGINAL REFERENCE NO.: 66:67a,70a

TITLE: Polarographic study of the effects of  $\gamma$ -radiation on cytosine

AUTHOR(S): Pleticha-Lansky, Roman; Weiss, Joseph J.

CORPORATE SOURCE: Univ. Newcastle-upon-Tyne, UK

SOURCE: Analytical Biochemistry (1966), 16(3), 510-22

CODEN: ANBCA2; ISSN: 0003-2697

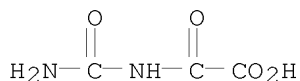
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Polarographic studies of the effects of  $\gamma$ -radiation on cytosine supplementing the Ekert-Monier scheme (Nature 188, 309 (1960)) showed that isobarbituric acid underwent further radiation-induced reactions. The temporary yellow-green color and the green fluorescence were ascribed to

the formation of 4,4'-diisobarbituric acid. Further radiolytic products of isobarbituric acid were isodialuric and dialuric acids. The easy oxidation of dialuric acid led to the formation of alloxan and subsequently to the system dialuric acid + alloxan .dblharw. alloxantin. With increasing radiation dose, parabanic acid was also formed, probably as an oxidative product of alloxanic acid formed by a benzilic acid type of rearrangement of alloxan. However, parabanic acid underwent hydrolysis, yielding oxaluric acid. Above a radiation dose of  $5 \times 10^{20}$  ev. ml<sup>-1</sup>, the overall effects were ring opening and hydrolytic formation of simple aliphatic compds., with the solution turning colorless. 28 references.

IT 585-05-7  
 RL: BIOL (Biological study)  
 (from isobarbituric acid after  $\gamma$ -irradiation)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)

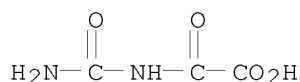


L6 ANSWER 76 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1966:474750 CAPLUS  
 DOCUMENT NUMBER: 65:74750  
 ORIGINAL REFERENCE NO.: 65:13997d-g  
 TITLE: Low spin ferric hemoglobin complexes  
 AUTHOR(S): Harris, Gilda  
 CORPORATE SOURCE: Stanford Univ., Stanford, CA  
 SOURCE: Theoretica Chimica Acta (1966), 5(5), 379-97  
 CODEN: TCHAAM; ISSN: 0040-5744  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A calcn. has been made of the energy eigenfunctions and eigenvalues of low-spin ferric ion in complexes with a strong cubic crystal field including the effects of tetragonal and rhombic distortions and of spin-orbit coupling among the ground state components and with excited states. Using the resultant, spin-orbit coupled eigenfunctions as a basis set, the magnetic susceptibility, the components of magnetic field energy, and the lattice and valence contributions to an elec. field gradient at the iron nucleus were all calculated as a function of rhombic, tetragonal, and spin-orbit coupling strength used as parameters: R, u, and  $\delta$ . All of the calculated results agree reasonably well with exptl. for the values of parameters R = 1000 cm.<sup>-1</sup> u = 2000 cm.<sup>-1</sup>, and the free ion value  $\delta$  = 420 cm.<sup>-1</sup> These values of parameters were selected for the excellent fit they gave of the calculated values of g<sub>x</sub>, g<sub>y</sub>, and g<sub>z</sub> compared with the exptl. ones obtained from single crystal ESR of ferriHb azide. With them, a value of 2.29  $\mu$ B was calculated for the effective magnetic moment compared to the exptl. value of 2.35. The total field gradient calculated under the same conditions predicts a nuclear quadrupole moment Q in the range of 0.107-0.127 barns, which is smaller than the range predicted from the high spin ferric ion results. Reasons for the discrepancy are discussed. 16 refs.

IT 13188-21-1  
 (Derived from data in the 7th Collective Formula Index (1962-1966))  
 RN 13188-21-1 CAPLUS  
 CN Oxaluric acid, monoammonium salt (8CI) (CA INDEX NAME)





● NH<sub>3</sub>

L6 ANSWER 77 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1965:18495 CAPLUS

DOCUMENT NUMBER: 62:18495

ORIGINAL REFERENCE NO.: 62:3338g-h,3339a

TITLE: Effects of metabolites and antimetabolites on the sporulation of *Peronospora tabacina* on tobacco leaf disks

AUTHOR(S): Shepherd, C. J.; Mandryk, M.

CORPORATE SOURCE: Div. Plant Ind., C.S.I.R.O., Canberra

SOURCE: Australian Journal of Biological Sciences (1964), 17(4), 878-91

CODEN: AJBSAM; ISSN: 0004-9417

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The effects of 148 metabolites and antimetabolites on the sporulation of *P. tabacina* on leaf disks of *Nicotiana tabacum* var Virginia Gold were determined. Sporulation intensities of 68 + 104 - 153 + 104 conidia/sq. cm. leaf area are observed. Normal metabolites, with the exception of FAD, have slight although statistically significant effects on sporulation intensity. This observation suggests that inhibition-nutrition phenomena play no part in the sporulation process. Seven uracil analogs have an inhibitory effect on sporulation, and reversal of inhibition by uracil suggests the active involvement of this compound in sporulation. Canavanine at a final concentration of 120 γ/ml. completely inhibits sporulation. Reversal of canavanine inhibition by arginine, citrulline, and ornithine suggests the involvement of arginine and the functioning of an ornithine cycle in the sporulation system. White, instead of the normal blue, conidia are produced in the presence of a number of S-containing compds. It is suggested that this phenomenon

depends on

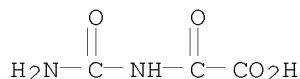
the chelating properties of these compds. toward Cu<sup>++</sup>, with the subsequent inactivation of tyrosinase activity in the conidia.

IT 585-05-7, Oxaluric acid

(*Peronospora tabacina* sporulation inhibition by)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 78 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1964:69852 CAPLUS

DOCUMENT NUMBER: 60:69852

ORIGINAL REFERENCE NO.: 60:12346d-e

TITLE: Purine metabolism of unicellular algae. I. Chromatographic detection of some purines, pyrimidines, and imidazoles by their mercuric complexes

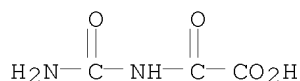
AUTHOR(S): Ammann, Elizabeth C. B.; Lynch, Victoria H.

CORPORATE SOURCE: Lockheed Missiles & Space Co., Palo Alto, CA

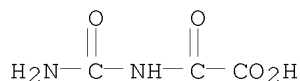
SOURCE: Analytical Biochemistry (1964), 7(4), 387-92

CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB A mercuric acetatediphenylcarbazon spray test for the identification of mixts. of xanthenes and uric acids was found to apply to other purines, to some pyrimidines and imidazoles, and to other cyclic N compds. containing an NH group cross-conjugated with 2 unsatd. groups. These compds. may be conveniently divided into 2 categories; (1) compds. which react with the spray test and which can also be detected by ultraviolet examination (hypoxanthine, xanthine, uric acid, guanine, adenine, orotic acid, violuric acid, and creatinine); (2) compds. which are not detected with the ultraviolet lamp in small quantities (10  $\gamma$ ) but which are stained with the spray (allantoin, hydantoin, parabanic acid, cyanuric acid, and alloxan). The chemistry of the reaction is discussed. This spray technique should be applicable for investigating the metabolism of purines in plants and animals.  
 IT 585-05-7, Oxaluric acid  
 (detection of)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 79 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1964:24542 CAPLUS  
 DOCUMENT NUMBER: 60:24542  
 ORIGINAL REFERENCE NO.: 60:4394h, 4395a  
 TITLE: Oxamic transcarbamylase of Streptococcus allantoicus  
 AUTHOR(S): Bojanowski, R.; Gaudy, Elizabeth; Valentine, R. C.; Wolfe, R. S.  
 CORPORATE SOURCE: Univ. of Illinois, Urbana  
 SOURCE: Journal of Bacteriology (1964), 87(1), 75-80  
 CODEN: JOBAA; ISSN: 0021-9193  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB An improved colorimetric assay for carbamyl oxamate, which allows the precise measurement of the activity of oxamic transcarbamylase, has been developed. Activity is maximum over the pH range 8.3-8.7. A cation requirement is satisfied by  $2.5 \times 10^{-3}\text{M}$   $\text{Mg}^{++}$  or  $\text{Mn}^{++}$ . The equilibrium constant for the phosphorylisis of carbamyl oxamic acid is 1.6, corresponding to a neg. free energy change of -285 cal./mole.  
 IT 585-05-7, Oxaluric acid  
 (determination of)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 80 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1963:42843 CAPLUS  
 DOCUMENT NUMBER: 58:42843  
 ORIGINAL REFERENCE NO.: 58:7335d  
 TITLE: Biosynthesis of carbamoyl oxamic acid  
 AUTHOR(S): Valentine, R. C.; Wolfe, R. S.  
 CORPORATE SOURCE: Univ. of Illinois, Urbana  
 SOURCE: Biochemical and Biophysical Research Communications (1960), 2, 384-7

From: Biol. Abstr. 36, Abstr. No. 11126(1961).

CODEN: BBRCA9; ISSN: 0006-291X

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

AB The major products of the fermentation of allantoin by *Streptococcus allantoicus* are ammonia, urea, oxamic acid, and CO<sub>2</sub>. Since the organism cannot convert urea to ammonia, it was concluded earlier that at least one of the ureido groups of allantoic acid is decomposed before being separated from the 2-carbon chain. An energy-yielding step could be the decomposition of this ureido group. The reaction may serve then as a primary energy source in *S. allantoicus*.

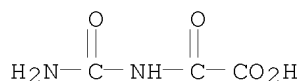
IT 585-05-7P, Oxaluric acid

RL: PREP (Preparation)

(formation from allantoin by *Streptococcus allantoicus*)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 81 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:471290 CAPLUS

DOCUMENT NUMBER: 57:71290

ORIGINAL REFERENCE NO.: 57:14218e-f

TITLE: Germination of conidia of *Peronospora tabacina*. I.  
Germination in vitro

AUTHOR(S): Shepherd, C. J.

CORPORATE SOURCE: Div. Plant Ind., C.S.I.R.O., Canberra

SOURCE: Australian Journal of Biological Sciences (1962), 15, 483-508

CODEN: AJBSAM; ISSN: 0004-9417

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

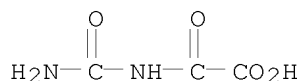
AB Washed conidia germinated poorly or not at all in H<sub>2</sub>O, but germinated in presence of riboflavine. Rate of germination in liquid suspension was enhanced by C and N sources, phosphate, Ca<sup>++</sup>, and Mg<sup>++</sup>. The effects of 141 metabolites on germination and germ-tube elongation were tested. Some analogs of purines and pyrimidines were inhibitory. Washing by centrifugation increased % germination, and presence of germination inhibitor in unwashed conidia is postulated. The optimum temperature for germination was in range 15-20°. The pH optimum was in range 5.5-8.0 on 2% agar and 6.5-8.0 in liquid suspension.

IT 585-05-7, Oxaluric acid

(effect on *Peronospora tabacina* germination)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 82 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

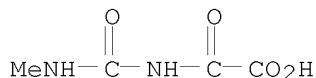
ACCESSION NUMBER: 1962:449317 CAPLUS

DOCUMENT NUMBER: 57:49317

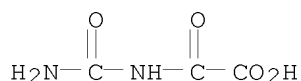
ORIGINAL REFERENCE NO.: 57:9846a-c

TITLE: Chemical structure of albomycin antibiotic. I.  
Isolation and identification of the pyrimidine base

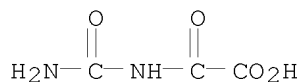
AUTHOR(S): Poddubnaya, N. A.; Lavrenova, G. I.; Krysin, E. P.;  
 Makevnina, L. G.  
 SOURCE: Zhurnal Obshchei Khimii (1961), 31, 3820-6  
 CODEN: ZOKHA4; ISSN: 0044-460X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB Paper electrophoresis of albomycin in 30% AcOH gave 3 fractions moving to the cathode; only the middle fraction was biol. active. A perpendicular paper chromatography in BuOH-H<sub>2</sub>O-AcOH separated the middle fraction into 3 subfractions of which only 1 was active. The content of the active material varies among samples so that numerical values are insignificant. Hydrolysis of albomycin in 20% HCl 24 hrs. gave a pyrimidine base identified as 1-methyluracil, m. 170-2°. This also formed from the active fraction isolated chromatographically above. Refluxing 2-ethylthio-6-hydroxypyrimidine with MeI in 95% EtOH in the presence of KOH gave 25% 1-methyl-2-ethylthio-6-hydroxypyrimidine, m. 78-9°, which heated with 20% HCl 1 day gave 1-methyluracil, m. 172-4° (Johnson and Heyl, CA 1, 2373). 6-Thiouracil and MeI in EtONa-EtOH gave 90% 2-hydroxy-3-methyl-6-methylthiopyrimidine, m. 115-20°, which with concentrated HCl gave 33% 3-methyluracil, m. 232°. These were oxidized with KMnO<sub>4</sub> to 6-methyloxaluric acid, m. 187°, along with some acetylurea and oxalic acid.  
 IT 89281-42-5P, Oxamic acid, (methylcarbamoyl)-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 89281-42-5 CAPLUS  
 CN Acetic acid, 2-[[ (methylamino)carbonyl]amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 83 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1962:34732 CAPLUS  
 DOCUMENT NUMBER: 56:34732  
 ORIGINAL REFERENCE NO.: 56:6592a-b  
 TITLE: Phenobarbital-C14 in the rat. II  
 AUTHOR(S): Glasson, B.; Benakis, A.  
 CORPORATE SOURCE: Univ. Geneva, Switz.  
 SOURCE: Helvetica Physiologica et Pharmacologica Acta (1961), 19, 323-34  
 CODEN: HPPAAL; ISSN: 0367-6242  
 DOCUMENT TYPE: Journal  
 LANGUAGE: French  
 AB cf. CA 53, 19146b. No exhaled C14O<sub>2</sub> was detected during the 24 hrs. following injection of phenobarbital-C14 in the rat. Seven different catabolites were radiochromatographically detected in the urine (details given). About 27% of the dose was excreted unchanged. Metabolites included p-hydroxyphenobarbital and its glucuronide, 2 or 3 unidentified compds., and the hitherto unreported 5-ethylbarbituric acid, parabanic acid, and oxaluric acid. There was no evidence of fission of the barbituric ring.  
 IT 585-05-7, Oxaluric acid  
 (as phenobarbital metabolite in urine)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



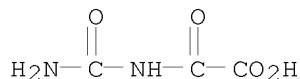
L6 ANSWER 84 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1961:138045 CAPLUS  
 DOCUMENT NUMBER: 55:138045  
 ORIGINAL REFERENCE NO.: 55:26107b-c  
 TITLE: Intermediates in anaerobic allantoid degradation by bacteria  
 AUTHOR(S): Vogels, G. D.  
 CORPORATE SOURCE: Technol. Univ., Delft, Neth.  
 SOURCE: Biochemische Zeitschrift (1961), 334, 457-61  
 CODEN: BIZEA2; ISSN: 0366-0753  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB Evidence has been obtained for the occurrence of oxaluric and allantoic acids as intermediates in the anaerobic breakdown of allantoin by 2 bacteria freshly isolated from ditch mud. The results indicate also that glyoxylic acid is an intermediate in the fermentation of allantoin. Glycine was found to be one of the end-products of this fermentation. A reaction scheme was proposed distinguishing between, on one hand, a hydrolytic and reductive pathway resulting in the formation of urea, glyoxylic acid, glycine and cell material via allantoic acid as an intermediate, and on the other hand, an oxidative pathway in which oxaluric and oxamic acids are formed via a dehydrogenation of allantoin.  
 IT 585-05-7P, Oxaluric acid  
 RL: PREP (Preparation)  
 (formation in allantoin metabolism by bacteria)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



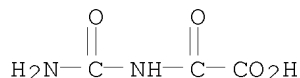
L6 ANSWER 85 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1961:87782 CAPLUS  
 DOCUMENT NUMBER: 55:87782  
 ORIGINAL REFERENCE NO.: 55:16627h-i,16628a-b  
 TITLE: Phosphorolysis of carbamoyloxamic acid  
 AUTHOR(S): Valentine, R. C.; Wolfe, R. S.  
 CORPORATE SOURCE: Univ. of Illinois, Urbana  
 SOURCE: Biochimica et Biophysica Acta (1960), 45, 389-91  
 CODEN: BBACAQ; ISSN: 0006-3002  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB cf. Biochim. Biophys. Research Commun. 2, 384(1960). The mechanism proposed for the decomposition of the ureido group of carbamoyloxamate (I) by Streptococcus allantoicus is: (1)  $\text{HO}_2\text{CCONHCONH}_2 + \text{inorg. phosphate} \rightarrow \text{H}_2\text{NCO} \cdot \text{apprx. P} + \text{HO}_2\text{CCONH}_2$ , and (2)  $\text{H}_2\text{NCO} \cdot \text{apprx. P} + \text{adenosine diphosphate} \rightarrow \text{NH}_3 + \text{CO}_2 + \text{adenosine triphosphate (ATP)}$ . Evidence supporting this mechanism is presented. ATP generation from I was coupled with acetate phosphorylation by means of an acetate kinase present in the enzyme preparation (loc. cit.). Acetyl phosphate was trapped as it was formed by  $\text{H}_2\text{NOH}$ . Under these conditions the equilibrium of reaction (1), which is towards the synthesis of I, was displaced since the ATP formed by reaction (2) was utilized in acetate activation. High concns. of neutral  $\text{H}_2\text{NOH}$  and acetate did not inhibit the reaction. Acethydroxamic acid formation from I required inorg. phosphate,  $\text{Mg}^{++}$ , acetate, adenosine diphosphate,  $\text{H}_2\text{NOH}$ , enzyme, and substrate. Inorg. phosphate played a catalytic role. Oxamate formation correlated well with I disappearance. Further evidence for the intermediary role of carbamoyl phosphate was the finding that I was an

active carbamoyl donor for the inorg. phosphate-dependent synthesis of citrulline from ornithine.

IT 585-05-7, Oxaluric acid  
(phosphorolysis by *Streptococcus allantoicus*)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)

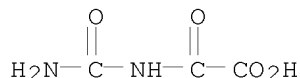


L6 ANSWER 86 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1960:51597 CAPLUS  
DOCUMENT NUMBER: 54:51597  
ORIGINAL REFERENCE NO.: 54:10159b-d  
TITLE: The metabolism of derivatives of barbituric acid. III.  
The metabolism of Phanodorn in the rat  
AUTHOR(S): Goldschmidt, St.; Koss, Fr. W.  
CORPORATE SOURCE: Tech. Hochschule, Munich, Germany  
SOURCE: Z. physiol. Chem. (1959), 316, 224-32  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB cf. C.A. 50, 7815a. Phanodorn-2-C14, (200 mg./kg. in 0.05N NaOH) was given to rats by means of an esophageal tube. Its excretion in feces as well as urine was measured and C14O2 determined in expired air. The metabolites of the drug were separated by paper chromatography and their structures elucidated. Almost all of the radioactivity of the drug was excreted within 70 hrs., mostly in the urine. Phanodorn as such and 4 of its metabolites were isolated. They were: oxaluric acid, 5-ethylbarbituric acid (I), 5-ethyl-5-(3-oxo-1-cyclohexenyl)barbituric acid (II), and 5-ethyl-5-(3-hydroxy-1-cyclohexenyl)barbituric acid (III).  
IT 585-05-7, Oxaluric acid  
(as Phanodorm metabolite)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 87 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1956:15975 CAPLUS  
DOCUMENT NUMBER: 50:15975  
ORIGINAL REFERENCE NO.: 50:3225b-c  
TITLE: The properties of interrelation of oxaluric and parabanic acids  
AUTHOR(S): Andrews, James C.; Sell, Irl T.  
CORPORATE SOURCE: Univ. of North Carolina, Chapel Hill  
SOURCE: Archives of Biochemistry and Biophysics (1955), 56, 405-11  
CODEN: ABBIA4; ISSN: 0003-9861  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB Conditions for the hydrolysis of parabanic (I) to oxaluric acid (II) and to urea and (CO2H)2 were studied by means of both titration and ultraviolet absorption spectra data. These show that at room temperature free I slowly changes to II whereas the salts of I change to II in a few min. The splitting of II to (CO2H)2 and urea is a slower process. I behaves as a monobasic acid with a pK value of 6.10. (CO2H)2 also shows only 1

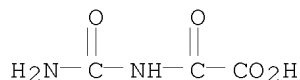
inflection of its titration curve at an approx. pH of 2.0.  
 IT 585-05-7, Oxaluric acid  
 (and salts)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 88 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1955:43214 CAPLUS  
 DOCUMENT NUMBER: 49:43214  
 ORIGINAL REFERENCE NO.: 49:8351f-h  
 TITLE: A comparative study of the end-products of uric acid  
 oxidation by peroxidases  
 AUTHOR(S): Canellakis, E. S.; Tuttle, Alice L.; Cohen, Philip P.  
 CORPORATE SOURCE: Univ. of Wisconsin, Madison  
 SOURCE: Journal of Biological Chemistry (1955), 213,  
 397-404  
 CODEN: JBCHA3; ISSN: 0021-9258  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. preceding abstrs. The oxidative decomposition of uric acid-2-C14 and  
 uric

acid-8-C14 by a catalase-EtO2H system and by systems of  
 lactoperoxidase-H2O2, verdoperoxidase-H2O2, and horseradish-H2O2 was  
 studied at neutrality. The catalase-EtO2H system oxidizes uric acid  
 beyond the allantoin stage. Among the labeled end-products of uric  
 acid-2-C14 oxidation are urea, allantoin, carbonyl diurea, oxalyl diurea,  
 cyanuric acid, oxonic acid, and CO2. Uric acid-8-C14 yields in addition  
 labeled parabanic acid and oxaluric acid. The lactoperoxidase-H2O2-borate  
 system yields urea, allantoin, 4,5-dihydroxy-5-ureido-2-imidazolidinone-4-  
 carboxylic acid, and alloxanic acid in contrast to the  
 verdoperoxidase-H2O2-phosphate and horseradish peroxidase-H2O2-phosphate  
 systems, which yield only urea and allantoin. The relation of these  
 systems, their possible biol. significance, and some aspects of the  
 mechanism of uric acid oxidation are discussed.

IT 585-05-7, Oxaluric acid  
 (from uric acid oxidation)  
 RN 585-05-7 CAPLUS  
 CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



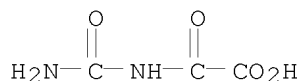
L6 ANSWER 89 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1954:27758 CAPLUS  
 DOCUMENT NUMBER: 48:27758  
 ORIGINAL REFERENCE NO.: 48:4974g-h  
 TITLE: The infrared spectra of the amides of oxalic acid in  
 the region between 3 and 6  $\mu$   
 AUTHOR(S): Chouteau, Jacques  
 CORPORATE SOURCE: Fac. sci., Marseille  
 SOURCE: Bulletin de la Societe Chimique de France (   
 1953) 1148-51  
 CODEN: BSCFAS; ISSN: 0037-8968  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB The infrared spectra are presented for unsubstituted oxamides, N-substituted oxamic acids, N,N'-substituted oxamides, and the imides of diacids. A comparison of these spectra permits the interpretation of structural analogs.

IT 585-05-7, Oxaluric acid  
(spectrum of)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 90 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1952:65842 CAPLUS

DOCUMENT NUMBER: 46:65842

ORIGINAL REFERENCE NO.: 46:10958h-i,10959a

TITLE: Polarographic behavior of parabanic, oxonic, and oxaluric acids

AUTHOR(S): Hladik, Vl.

CORPORATE SOURCE: Charles Univ., Prague

SOURCE: Sbornik Mezinarod. Polarog. Sjezdu Praze, 1st. Congr. (1951), (Pt. I.), Proc. 680-6;686-94

DOCUMENT TYPE: Journal

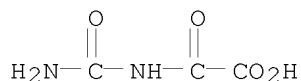
LANGUAGE: Russian/German

AB Parabanic acid is polarographically reducible; 3 different waves are obtained for the undissocd. acid and the uni- and bivalent anions, resp. Its dissociation consts. are  $6 + 10^{-7}$  and  $1.59 + 10^{-11}$  at  $20^\circ$ . Oxaluric acid is reduced polarographically in 2 steps at such neg. potentials that the wave height and half-wave potentials can only be estimated; its dissociation constant is  $1 + 10^{-5}$  at  $18^\circ$ . Oxonic acid (allantoxanic acid) is more easily reduced than parabanic acid; it also shows the 3 different waves. Its dissociation consts. are  $1.6 + 10^{-5}$  and  $8 + 10^{-7}$  at  $18^\circ$ . The polarographic data which served to calculate the dissociation consts. were also used to determine the reaction-velocity consts. of the hydrolysis of parabanic and oxaluric acids.

IT 585-05-7, Oxaluric acid  
(polarography of)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 91 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1938:18268 CAPLUS

DOCUMENT NUMBER: 32:18268

ORIGINAL REFERENCE NO.: 32:2591h-i,2592a

TITLE: Biology of oxalic acid. II. Oxalogenic compounds of urine

AUTHOR(S): Flaschentrager, Bonifaz; Muller, Paul B.

SOURCE: Z. physiol. Chem. (1938), 251, 61-9

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

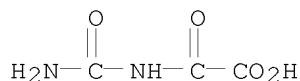
AB Continued extraction of acidified urine with Et<sub>2</sub>O after 2 hrs. yields regularly 0.25-0.55 mg.% (CO<sub>2</sub>H)<sub>2</sub> per hr. Tests show that oxaluric, parabanic, uric and ascorbic acids, allantoin, alloxan, creatinine and glucose yield more



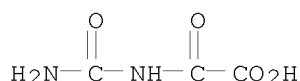
or less, and glycollic acid and glycine yield no oxalic acid in the determination

The quantities of oxaluric and parabanic acids and alloxan in urine are not sufficient to account for the extra oxalic acid formed. Oxalic acid is decomposed by H<sub>2</sub>O<sub>2</sub> at 90° and tissue pH, it is not affected by HgO + NaOH. If urine is treated with NaOH and HgCl<sub>2</sub> extra oxalic acid is formed. Under these conditions considerable quantities of oxalic acid are formed from glycollic and uric acids, glycine and creatinine.

IT 585-05-7, Oxaluric acid  
(in urine)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)

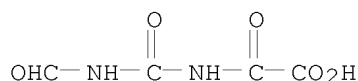


L6 ANSWER 92 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1935:36637 CAPLUS  
DOCUMENT NUMBER: 29:36637  
ORIGINAL REFERENCE NO.: 29:4741e-g  
TITLE: Action of hydrazine on cyclic ureides (parabanic acid)  
AUTHOR(S): Fosse, Richard; Thomas, Paul-Emile; de Graeve, Paul  
SOURCE: Compt. rend. (1935), 200, 1260-4  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
GI For diagram(s), see printed CA Issue.  
AB Parabanic acid (I), treated with (NH<sub>2</sub>)<sub>2</sub>, gave NH<sub>2</sub>CONH(CO)<sub>2</sub>NHNH<sub>2</sub> (II), m. 198° (decomposition); with PhNHNH<sub>2</sub> it gave NH<sub>2</sub>CO-NH(CO)<sub>2</sub>NHNHPh. I, treated with xanthidrol (III), gave CO.NR.CO.NR.CO (R = xanthyl), m. 214°. II, treated with III, gave RNHCONH(CO)<sub>2</sub>NHNH<sub>2</sub>; with BzH, PhCH:NNH(CO)<sub>2</sub>NHCONH<sub>2</sub>, m. 215° (decomposition); with CH<sub>2</sub>O, CH<sub>2</sub>:NNH(CO)<sub>2</sub>NHCONH<sub>2</sub>, m. 212° (decomposition); with AcH, MeCH:NNH(CO)<sub>2</sub>NHCONH<sub>2</sub>, m. 224° (decomposition).  
IT 585-05-7, Oxaluric acid  
(hydrazides)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 93 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1932:9234 CAPLUS  
DOCUMENT NUMBER: 26:9234  
ORIGINAL REFERENCE NO.: 26:1034c-d  
TITLE: Studies on the physiology of pyrimidines. V. The effects of certain pyrimidines on the sulfur metabolism of the dog  
AUTHOR(S): Stekol, Jakob A.; Cerecedo, Leopold R.  
SOURCE: Journal of Biological Chemistry (1931), 93, 275-82  
CODEN: JBCHA3; ISSN: 0021-9258  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB Isobarbituric, isodialuric and formyloxaluric acids, when fed to dogs, were partly metabolized to urea, and in the case of isobarbituric acid partly excreted as "ethereal" sulfate. In each case the excretion of neutral S was partly or wholly inhibited on the day after feeding the

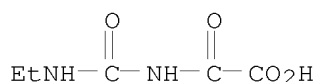
compound  
 IT 106055-61-2, Oxamic acid, N-formylcarbamyl-  
 (metabolism of)  
 RN 106055-61-2 CAPLUS  
 CN Acetic acid, 2-[[((formylamino)carbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 94 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1925:22575 CAPLUS  
 DOCUMENT NUMBER: 19:22575  
 ORIGINAL REFERENCE NO.: 19:2933c  
 TITLE: Oxidation of uric acid glycols  
 AUTHOR(S): Slotta, K. H.  
 SOURCE: Journal fuer Praktische Chemie (Leipzig) (1925  
 ), 110, 264-72  
 CODEN: JPCEAO; ISSN: 0021-8383  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB The glycols (10 g.) were oxidized with 80 cc. perhydrol (Merck) at room temperature Uric acid glycol after 4 days gave 42% of NH<sub>4</sub> oxalurate. 9-Methyluric acid glycol gave 74% of NH<sub>4</sub> methyloxalurate. 9-Ethyluric acid glycol gave only 0.32 g. NH<sub>4</sub> ethyloxalurate, m. 232° (decomposition). 7,9-Dimethyluric acid glycol gave 50% of (CONHMe)<sub>2</sub>, m. 217°, while the 7,9-di-Et derivative gave 2.1 g. (CONHEt)<sub>2</sub>, m. 180°.

IT 105918-81-8P, Oxaluric acid, ethyl-, ammonium salt  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 105918-81-8 CAPLUS  
 CN Acetic acid, 2-[[((ethylamino)carbonyl)amino]-2-oxo-, ammonium salt (1:1)  
 (CA INDEX NAME)



L6 ANSWER 95 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1924:13537 CAPLUS  
 DOCUMENT NUMBER: 18:13537  
 ORIGINAL REFERENCE NO.: 18:1816e-i,1817a  
 TITLE: Action of alkali on substituted uric acids I.  
 1,3-Dimethyl-9-phenyluric acid  
 Gatewood, Elizabeth Stuart  
 AUTHOR(S): Gatewood, Elizabeth Stuart  
 SOURCE: Journal of the American Chemical Society (1923  
 ), 45, 3056-64  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 18:13537

GI For diagram(s), see printed CA Issue.

AB 1,3-Dimethyl-9-phenyluric acid (I) is decomposed only very slowly by 4 N alkali at room temperature; at 100° with more dilute alkali, the decomposition

is more rapid and with 4 N alkali it is instantaneous; the products are MeNH<sub>2</sub>, CO<sub>2</sub> and 3-phenylisohydantoin-5-carboxylic methylamide, NH.CO.NPh.C(OH):CCONHMe (II). When warmed with alkali, or even on standing about an hr. with cold alkali, II decomps. completely into PhNHCONH<sub>2</sub>, MeNH<sub>2</sub>, (CO<sub>2</sub>H)<sub>2</sub> and HCO<sub>2</sub>H; the PhNHCONH<sub>2</sub> seps. after only 15 min. but no (CO<sub>2</sub>H)<sub>2</sub> can yet be detected at this point unless the solution is first warmed, indicating that its formation is due to a secondary reaction; probably OHCCO<sub>2</sub>H is first formed and changes into (CO<sub>2</sub>H)<sub>2</sub> and HOCH<sub>2</sub>CO<sub>2</sub>H when heated or allowed to stand with the alkali. With H<sub>2</sub>O<sub>2</sub> in dilute alkaline solution II yields 3-phenyl-5-hydroxyhydantoin-5-carboxylic methylamide, NH.CO.NPh.CO.C(OH)CONHMe (III), which is instantly decomposed by cold alkali into PhNHCONH<sub>2</sub> and HO<sub>2</sub>CCOCONHMe (IV) and on boiling is further decomposed into MeNH<sub>2</sub>, PhNHCONH<sub>2</sub> and CO(CO<sub>2</sub>H)<sub>2</sub> (V). II (1.2-1.4 g. from 2 g. I in 100 cc. of 4 N NaOH slowly heated to boiling, boiled 0.5 min., cooled slightly, acidified with HCl and allowed to stand), rectangular plates, α 1.571, γ 1.629, m. 249-50°, gives with boiling Ac<sub>2</sub>O a substance m. 185-7°, does not react with PhNCO at 165° or in alkaline solution at 0°. III (0.6 g. from 1 g. II in 12 cc. H<sub>2</sub>O with 2.9 g. KOH and 70 cc. of 3% H<sub>2</sub>O<sub>2</sub> kept 5 min. below 10° and then acidified with HCl), rectangular plates, α 1.545, γ 1.583, m. 194-5°; the mother liquors yield a substance separating in needles, α 1.556, γ 1.695, m. 188-90°. The phenylhydrazone of V seps. in needles, α 1.459, γ 1.800, m. 165°; that of IV in hexagonal plates, α 1.600, γ 1.715, m. 167° (Torrey, Ber. 31, 2162 (1898), gives 158°). Et phenyloxalurate (4.7 g. from 5 g. NH<sub>2</sub>COCO<sub>2</sub>Et and 10 g. PhNCO heated 1 hr. at 110-2°), m. 125-6° (gas evolution), seps. in 2 crystalline forms, α 1.590, γ 1.680, and α 1.675, γ 1.755, resp.; 1 g. allowed to stand in H<sub>2</sub>O 0.5 hr. with 1 g. of 33% MeNH<sub>2</sub> gives 0.74 g. of the methylamide, m. 210-5°, α 1.595, γ 1.700, instantly decompd. by cold 4 N NaOH into PhNHCONH<sub>2</sub>, (CO<sub>2</sub>H)<sub>2</sub> and MeNH<sub>2</sub>. 1,7-Di-methyl-9-phenylpseudouric acid (8 g. from 5 g. 1,7-dimethyluramil in 60 cc. of N KOH treated at 0-2° in the course of 0.5 hr. with 3.8 g. PhNCO), turns pink 160°, light yellow 210°, m. 220°, dissolves in about 350 parts H<sub>2</sub>O, seps. in hexagonal plates, α 1.555, γ 1.695; 5 g. boiled in 1 l. of 20% HCl until crystallization begins and concentrated yields 3.8 g.

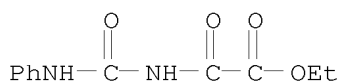
1,7-dimethyl-9-

phenyluric acid, rectangular and hexagonal plates, α 1.540, γ 1.755, does not m. 280°, is unchanged by boiling 10 min. with 4 N alkali, is also obtained in 0.5 g. yield, together with 0.1 g. of the 1,3,7-Me<sub>3</sub> acid, from 1 g. of 7-methyl-9-phenyluric acid with 2 g. Me<sub>2</sub>SO<sub>4</sub> in 2 N NaOH.

IT 221391-80-6P, Oxaluric acid, phenyl-, ethyl ester  
RL: PREP (Preparation)  
(preparation of)

RN 221391-80-6 CAPLUS

CN Acetic acid, oxo[[ (phenylamino)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 96 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1924:3772 CAPLUS

DOCUMENT NUMBER: 18:3772

ORIGINAL REFERENCE NO.: 18:531a-i,532a-c

TITLE: Oxidation of uric acid

AUTHOR(S): Biltz, Heinrich; Schauder, Hans

SOURCE: Journal de Physiologie (Paris, 1946-1992) (1923), 106, 108-72

CODEN: JOPHAN; ISSN: 0021-7948

DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB The number of oxidation products of uric acid (I) is very large; this is due in part to the characteristic unsym. formula of uric acid and also to the different action of various oxidizing agents. The oxidation products, however, depend more upon the nature of the solution than upon the sp.

nature

of the oxidizing agent, i. e., the same reagent will give different products, depending on whether the reaction is carried out in acid, alkaline or neutral medium. The mechanism of the alkaline oxidation is fairly well known; the formation of alloxan (II) and parabanic acid (III) by acid oxidation is not so well understood. Oxidation of 10 g. I in 300 cc. H<sub>2</sub>O containing 9 g. KOH with 16.3 g. KMnO<sub>4</sub> (2.6 atoms O) in 4% solution

acidified

with 20 cc. AcOH, gave 22% K oxalurate (see below) (IV), 14% CO(NH<sub>2</sub>)<sub>2</sub> isolated as the HNO<sub>3</sub> salt (V), and 1.6-1.8 g. oxalyldiureide (VI). The reaction proceeds in the same way with 2 atoms O, the extra 0.6 atom used above accounting for the side reactions. If the oxidation is carried out with solid I suspended in 20% AcOH (by volume), there result 16% IV, 22% V and 0.5 g. impure VI. Even with 1 atom O, (CO<sub>2</sub>H)<sub>2</sub> is the principal oxidation product. Oxidation of 5 g. I by 8 g. K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and 6 g. AcOK in 50 cc. H<sub>2</sub>O at 100° gave about 1 g. II. If 2 atoms O are used, there are formed IV and VI. In the presence of CO<sub>2</sub>, I is oxidized in the same manner as in AcOH. A neutral oxidation with KMnO<sub>4</sub> or K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> cannot be carried out because the 1 develops alkali, the other acid immediately after the reaction starts. Therefore H<sub>2</sub>O<sub>2</sub> was used. Boiling 2 g. I, 1 cc. perhydrol and 30 cc. H<sub>2</sub>O and adding H<sub>2</sub>O<sub>2</sub> until 5 cc. have been used, there result 0.4 g. CO(NHCONH<sub>2</sub>)<sub>2</sub> and 0.05 g. cyanuric acid; the same products result in AcOH. In the presence of H<sub>2</sub>SO<sub>4</sub>, KMnO<sub>4</sub> and K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> give II, though the yield is very small. When 2 g. I, 30 cc. H<sub>2</sub>O, 5 cc. 2 N HCl and 1 cc. H<sub>2</sub>O<sub>2</sub> are heated 25 min. (solution), and the solution is

filtered

and concentrated on the H<sub>2</sub>O bath, there results 52% III. This is a very suitable method for its preparation. A decrease in the amount of HCl causes

a

decided decrease in the yield. KMnO<sub>4</sub> equivalent to 1 atom O, acting on 3 g. uric acid 4,5-glycol in dilute AcOH at 0° for 2-3 weeks, gave 0.9 g. IV; at 100° this yield is decreased to 0.4 g. Since the reaction proceeds so slowly, this glycol is excluded as an intermediate product in the formation of IV from I. The 9-Me derivative under the same conditons

gave

only a few cg. of methyloxaluric acid. The 7,9-Me<sub>2</sub> derivative gave a very small and variable yield of dimethylparabanic acid. II is oxidized to IV in AcOH, KMnO<sub>4</sub> giving a 47 and H<sub>2</sub>O<sub>2</sub> a 61% yield. The latter method (2 g. II.H<sub>2</sub>O and 4 cc. perhydrol 10 min. on the H<sub>2</sub>O bath) is a very suitable method for preparing small amts. of the free acid of IV. IV is also

obtained

in about 60% yields by oxidation in AcOH (2 days at room, 15 min. at boiling temperature), the mother liquor containing a corresponding amount of V. These

products are not the intermediate product in the formation of IV from I, because their oxidation proceeds too slowly. The hypothetical hydroxyacetylenediureincarboxylic acid [present in the alkaline oxidation

of I

by KMnO<sub>4</sub> (1 atom)] on oxidation with a second atom of O in AcOH, however, yields 46% IV and 30% V, and some VI. IV contains 1 mol. H<sub>2</sub>O which is completely removed only at 120°. The free acid (VII) is best obtained by dissolving 2.5 g. IV in 25 cc. boiling H<sub>2</sub>O, cooling to 75°, acidifying with 5 cc. concentrated HCl and cooling in ice H<sub>2</sub>O, the yield being 85%. It decomp. 208-10°; at 95° water dissolves 2.6%; because of its instability, the loss on crystallization

from H<sub>2</sub>O

is about 35%. The NH<sub>4</sub> salt is prepared by rubbing finely pulverized VII with half-concentrated NH<sub>4</sub>OH, filtering, washing with a little cold H<sub>2</sub>O and crystallizing from 4 parts boiling H<sub>2</sub>O; it decomp. 242-4°. Me oxalurate, m. 192° (decomposition), from VII and CH<sub>2</sub>N<sub>2</sub>; solubility in AcOH,

about 3%. It is more stable towards H<sub>2</sub>O than VII, can be saponified by AcOK but is decomposed by KOH. The methylamide (VIII), decomposing 251-3°, results from the Me ester and MeNH<sub>2</sub> or by the oxidation of 1,3-dimethyluric acid. VII is decomposed by acids or alkalies, giving CO(NH<sub>2</sub>)<sub>2</sub> and (CO<sub>2</sub>H)<sub>2</sub>. Three g. VII in 11 cc. H<sub>2</sub>O boiled 15 min., give 1 g. C<sub>2</sub>H<sub>2</sub>O<sub>4</sub>.2CO(NH<sub>2</sub>)<sub>2</sub> and 0.5 g. C<sub>2</sub>H<sub>2</sub>O<sub>4</sub>.NH<sub>4</sub>.C<sub>2</sub>H<sub>2</sub>O<sub>4</sub>.2H<sub>2</sub>O under other conditions a mixture of these, m. 130-75°, results. On mixing mol. amts. of C<sub>2</sub>H<sub>2</sub>O<sub>4</sub> and CO(NH<sub>2</sub>)<sub>2</sub> there ppts. C<sub>2</sub>H<sub>2</sub>O<sub>4</sub>.2CO(NH<sub>2</sub>)<sub>2</sub>, also obtained after short heating, but if the boiling is continued 2 hrs. there results C<sub>2</sub>O<sub>4</sub>(NH<sub>4</sub>)<sub>2</sub>.H<sub>2</sub>O. Attempts to prepare Lubavin's urea oxalate (Ann., Suppl. 8, 83) failed and it is probable that the compound does not exist. Oxidation of 1,3-dimethyluric acid with alkaline KMnO<sub>4</sub> gives a little IV and some dimethyloxamide (IX). Oxidation with alkaline KMnO<sub>4</sub> (1 atom O)

followed

by the addition of AcOH and a 2nd atom O gave from 10 g. acid, 1.3 g. IV, 0.4

g. dimethylparabanic acid and 0.3 g. IX. There was also found 0.15-0.2 g. VIII. The yield of oxidation products with AcOH was very small. Oxidation with H<sub>2</sub>O<sub>2</sub> in alkaline solution gave a new product, needles, m. 215°. Oxidation of 10 g. 3,7-dimethyluric acid in alkaline medium with 1 atom of O gave 0.06 g. 1,8-dimethylallantoin, and an acid, C<sub>6</sub>H<sub>5</sub>O<sub>5</sub>N<sub>3</sub>, long prisms, m. 212° (decomposition), the K salt of which forms thick rhombic plates and gradually decomps. above 275°. Oxidation of I with Cl in the presence of AcONa does not give II, nor could any definite product be isolated. If the oxidation of the uric acids to alloxans proceeds through the glycols, then the latter in the presence of mineral acids should yield the corresponding alloxans. This is not the case (the 1,3-Me<sub>2</sub> derivative is an exception). Chloro- or hydroxypseudouric acid is easily transformed into II in acid solution The "chloraluric acid" of

Schiel

(Ann. 112, 78) consists of a mixture of NH<sub>4</sub>Cl and III. Attempts to repeat the work of Gibbs (Ber. 2, 341) on the preparation of "stryphnic acid" by

the

action of KNO<sub>2</sub> and mineral acids on I gave allantoin, VII, and (CO<sub>2</sub>H)<sub>2</sub>, but his acid was not observed. Similarly the work of Sokoloff (Z. fur Chemical 5, 78(1869)), who claims the preparation of "urinilic acid" could

not be

duplicated. NO does not react upon a mixture of I and H<sub>2</sub>O. The use of a mixture of NO and NO<sub>2</sub> (less NO<sub>2</sub>) gives a mixture of uric acid glycol, III

and

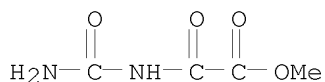
a little II. A mixture rich in NO<sub>2</sub> gives xanthine, II, III and a little C<sub>2</sub>H<sub>2</sub>O<sub>4</sub>.

IT 530084-26-5P, Oxaluric acid, methyl ester

RL: PREP (Preparation)  
(preparation of)

RN 530084-26-5 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo-, methyl ester (CA INDEX NAME)



L6 ANSWER 97 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1921:8150 CAPLUS

DOCUMENT NUMBER: 15:8150

ORIGINAL REFERENCE NO.: 15:1546g-i

TITLE: The determination of oxalic acid and oxaluric acid in urine and feces

AUTHOR(S): Bau, A.

SOURCE: Biochemische Zeitschrift (1921), 114, 221-57

CODEN: BIZEA2; ISSN: 0366-0753

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB A reagent for the determination of oxalic acid in urine is prepared as follows: (a)

a mixture of 330 g. of Na acetate and 300 cc. H<sub>2</sub>O is warmed to solution, cooled

and filtered if necessary. (b) 25 g. of crystallized CaCl<sub>2</sub> is dissolved in 50%

AcOH, put into a 500-cc. graduated flask and filled to the mark with (a). This solution is allowed to stand at 7° for 48 hrs. and is then filtered through a hard S. & S. filter. For the analysis of urine, a measured amount of the filtered specimen is taken, 1/6 its volume of the reagent is added and the whole is allowed to stand for 38 to 44 hrs. in the cold. The precipitate is filtered, washed, ashed, heated to whiteness, weighed and titrated with 0.1 N HCl. The presence of glucose or albumin in the urine does not interfere with the accuracy of the determination

Oxaluric

acid is not precipitated by the reagent. This latter compound is determined by 1st

changing it to oxalic acid by boiling with HCl and following the procedure outlined above. The determination of oxalic or oxaluric acid in feces is preceded

by defatting, and drying, after which a satisfactory extraction can be made with HCl. This extract is neutralized with NH<sub>4</sub>OH, buffered with a neutral solution of NH<sub>4</sub> citrate and the determination of oxalic acid is carried out

as

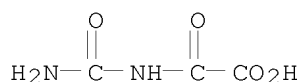
indicated.

IT 585-05-7, Oxaluric acid

(determination in urine and feces)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 98 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1906:64302 CAPLUS

DOCUMENT NUMBER: 0:64302

TITLE: A reagent for the identification of urea and certain other nitrogen compounds

AUTHOR(S): Fenton, Henry J. Horstman

SOURCE: Journal of the Chemical Society, Transactions (1903), 83, 187-190

CODEN: JCHTA3; ISSN: 0368-1645

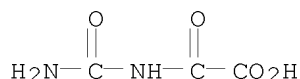
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB A considerable number of new derivatives of methylfurfural have been described. The starting point for the preparation of these compounds is the bromo-derivative, O:CH·C<sub>4</sub>H<sub>2</sub>O·CH<sub>2</sub>Br, or the corresponding chloro-derivative. These compounds are easily obtained by the action of the dry halogen acids on ketohexoses or on cellulose. Among the various compounds obtained from these derivatives, a condensation product was described with the formula C<sub>11</sub>H<sub>3</sub>O<sub>4</sub>. If the reagent be ground together with urea and the mixture treated with phosphorus oxychloride, acetyl chloride, or dry hydrogen chloride, a Prussian blue color was developed. In using the reaction as a test for urea, the solids are well mixed together, or if the substance to be examined is in solution, it is mixed with an alcoholic solution of the reagent and evaporated to dryness on the water-bath. The phosphorus oxychloride might be dissolved in an appropriate solvent, e.g., light petroleum, glacial acetic acid, or benzene. Preliminary analysis of the urea base indicated that it is formed by condensation of one molecule of the reagent C<sub>11</sub>H<sub>8</sub>O<sub>4</sub> with two molecules of urea, and if the other bases are similarly constituted, this

fact accounts for the necessity of the NH<sub>2</sub> group in the reacting nitrogen compound.

IT 585-05-7, Oxaluric acid  
(reagent for identification of urea and certain other nitrogen compounds)  
RN 585-05-7 CAPLUS  
CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 99 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1906:62899 CAPLUS

DOCUMENT NUMBER: 0:62899

TITLE: The action of phenylhydrazine on urea and some of its derivatives

AUTHOR(S): Skinner, Sidney; Ruhemann, S.

CORPORATE SOURCE: University Laboratory, Cambridge, Cambridge

SOURCE: Journal of the Chemical Society, Transactions (1888), 53, 550-558

CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

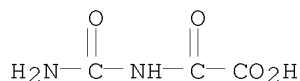
LANGUAGE: Unavailable

AB The compound diphenylcarbazine is produced when mixture of phenylhydrazine and ethylic carbamate is heated over a small flame. Heating equivalent quantities of monophenylcarbamide and phenylhydrazine and phenylhydrazine and monophenylthiocarbamide produced the substance diphenylsemicarbazide and phenylsemithiocarbamide, respectively. If a drop of dilute copper sulphate solution is added to a solution of any of these carbazides or semicarbazides, and intense coloration is produced. Biuret and phenylhydrazine, when heated, produced phenylurazole. An aqueous solution of mercuric chloride added to an alcoholic solution of the diphenylcarbazine gives diphenylcarbazine mercuriochloride. A solution of phenylhydrazine hydrochloride has no action on a solution of parabanic acid, but on adding sodium acetate to this mixture, phenylhydrazine parabanate is produced. Oxalurydrazide is produced when phenylhydrazide parabanate boiled with a very large excess of water is cooled. The reaction between alloxan in aqueous solution and phenylhydrazine hydrochloride in the presence of sodium acetate resulted to phenylhydrazine-alloxan. Phenyl-piperyl-thiocarbamide is a crystalline substance prepared by adding isothiocyanate to piperidine.

IT 585-05-7, Oxaluric acid  
(action of phenylhydrazine on urea and its derivatives)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)



L6 ANSWER 100 OF 100 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1906:48874 CAPLUS

DOCUMENT NUMBER: 0:48874

TITLE: The normal urine

AUTHOR(S): Platt, Charles

CORPORATE SOURCE: Chemical Laboratory, Hahnemann Medical College, Philadelphia

SOURCE: Journal of the American Chemical Society (1897), 19(5), 382-4

CODEN: JACSAT

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The various compilations existing as "Text-books of Urine Analysis" differ materially in their statements as to the average composition of a normal urine. Great variations have been found in the original figures, due not so much to errors of determination as to failure to secure representative samples for analysis. Normals determined for one nationality, or for one class of one nationality, are commonly applied indiscriminately to all without regard to fundamental differences in conditions. In view of this laxity in text-book statement, careful records of all urine analyses have been made with due attention to the age, sex, and health of the individuals supplying the samples. These figures are provided.

IT 585-05-7, Oxaluric acid  
(study of normal urine analysis)

RN 585-05-7 CAPLUS

CN Acetic acid, 2-[(aminocarbonyl)amino]-2-oxo- (CA INDEX NAME)

